Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis:
Version 6.6 Developers Manual

Brian M. Adams, Mohamed S. Ebeida, Michael S. Eldred, Gianluca Geraci, John D. Jakeman, Kathryn A. Maupin, Jason A. Monschke, Laura P. Swiler, J. Adam Stephens, Dena M. Vigil, Timothy M. Wildey
Optimization and Uncertainty Quantification Department

William J. Bohnhoff
Radiation Transport Department

Keith R. Dalbey
Mission Analysis and Simulation Department

John P. Eddy
System Readiness and Sustainment Technologies Department

Joseph R. Frye, Russell W. Hooper
Multiphysics Applications Department

Kenneth T. Hu
Validation and Uncertainty Quantification Department

Patricia D. Hough, Mohammad Khalil
Quantitative Modeling and Analysis Department

Elliott M. Ridgway
Data-driven and Neural Computing
Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185

Ahmad Rushdi
Electrical and Computer Engineering
University of California
One Shields Avenue
Davis, CA 95616-5294
Abstract

The Dakota toolkit provides a flexible and extensible interface between simulation codes and iterative analysis methods. Dakota contains algorithms for optimization with gradient and nongradient-based methods; uncertainty quantification with sampling, reliability, and stochastic expansion methods; parameter estimation with nonlinear least squares methods; and sensitivity/variance analysis with design of experiments and parameter study methods. These capabilities may be used on their own or as components within advanced strategies such as surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty. By employing object-oriented design to implement abstractions of the key components required for iterative systems analyses, the Dakota toolkit provides a flexible and extensible problem-solving environment for design and performance analysis of computational models on high performance computers.

This report describes the Dakota class hierarchies. It is derived from annotation of the source code and provides detailed class documentation, including all member functions and attributes.
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Chapter 1

Dakota Developers Manual

Author


1.1 Introduction

The Dakota software (http://dakota.sandia.gov/) delivers advanced parametric analysis techniques enabling quantification of margins and uncertainty, risk analysis, model calibration, and design exploration with computational models. Dakota contains algorithms for optimization with gradient and nongradient-based methods, uncertainty quantification with sampling, reliability, stochastic expansion, and interval estimation methods, parameter estimation with nonlinear least squares methods, and sensitivity/variance analysis with design of experiments and parameter study capabilities. (Solution verification and Bayesian approaches are also in development.) These capabilities may be used on their own or as components within advanced algorithms such as surrogate-based optimization, mixed integer nonlinear programming, mixed aleatory-epistemic uncertainty quantification, or optimization under uncertainty. By employing object-oriented design to implement abstractions of the key components required for iterative systems analyses, the Dakota toolkit provides a flexible problem-solving environment for design and performance analysis of computational models on high performance computers.

The Developers Manual focuses on documentation of Dakota design principles and class structures; it derives principally from annotated source code. For information on input command syntax, refer to the Reference Manual[1], and for more details on Dakota features and capabilities, refer to the Users Manual.

1.2 Overview of Dakota

In Dakota, the environment manages execution modes and input/output streams and defines the top-level iterator. This top-level iterator may be either a standard iterator or a meta-iterator. In the former case, the iterator identifies a model and the environment executes the iterator on the model to perform a single study. In the latter case, iterator recursions are present and sub-iterations may identify their own models. In both cases, models may contain additional recursions in the case of nested iteration or surrogate modeling. In a simple example, a hybrid meta-iterator might manage a global optimizer operating on a low-fidelity model that feeds promising design points into a local optimizer operating on a high-fidelity model. And in a more advanced example, a surrogate-based optimization under uncertainty approach would employ an uncertainty quantification iterator nested within an
optimization iterator and would employ truth models contained within surrogate models. Thus, iterators and models provide both stand-alone capabilities as well as building blocks for more sophisticated studies.

A model contains a set of variables, an interface, and a set of responses, and the iterator operates on the model to map the variables into responses using the interface. Each of these components is a flexible abstraction with a variety of specializations for supporting different types of iterative studies. In a Dakota input file, the user specifies these components through environment, method, model, variables, interface, and responses keyword specifications.

The use of class hierarchies provides a mechanism for extensibility in Dakota components. In each of the various class hierarchies, adding a new capability typically involves deriving a new class and providing a set of virtual function redefinitions. These redefinitions define the coding portions specific to the new derived class, with the common portions already defined at the base class. Thus, with a small amount of new code, the existing facilities can be extended, reused, and leveraged for new purposes. The following sections tour Dakota’s class organization.

1.2.1 Environment

Class hierarchy: Environment.

Environments provide the top level abstraction for managing different execution modes and managing input and output streams. Specific environments include:

- **ExecutableEnvironment**: the environment for execution of Dakota as a stand-alone application.
- **LibraryEnvironment**: the environment for execution of Dakota as an embedded library service.

1.2.2 Iterators

Class hierarchy: Iterator. Iterator implementations may choose to split operations up into run-time phases as described in Understanding Iterator Flow.

The iterator hierarchy contains a variety of iterative algorithms for optimization, uncertainty quantification, nonlinear least squares, design of experiments, and parameter studies. The hierarchy is divided into **MetaIterator**, **Minimizer**, and **Analyzer** branches.

The **MetaIterator** classes manage sequencing and collaboration among multiple methods with support for concurrent iterator parallelism. Methods include:

- **SeqHybridMetaIterator**: hybrid minimization using a set of iterators employing a corresponding set of models of varying fidelity. The sequential hybrid passes the best solutions from one method in as the starting points of the next method in the sequence.
- **CollabHybridMetaIterator**: hybrid minimization employing collaboration and sharing of response data among methods during the course if iteration. This class is currently a placeholder.
- **EmbedHybridMetaIterator**: hybrid minimization involving periodic use of a local search method for refinement during the iteration of an outer global method. This class is currently a placeholder.
- **ConcurrentMetaIterator**: two similar algorithms are available: (1) multi-start iteration from several different starting points, and (2) pareto set optimization for several different multi-objective weightings. Employs a single iterator with a single model, but runs multiple instances of the iterator concurrently for different settings within the model.

The **Minimizer** classes address optimization and deterministic calibration and are grouped into:
1.2. OVERVIEW OF DAKOTA

- Optimization: **Optimizer** provides a base class for gradient-based (e.g., CONMINOptimizer and SNL-LOptimizer) and derivative-free (e.g., NCSUOptimizer, JEGAOptimizer) optimization solvers. Most of these are wrappers for third-party libraries that implement the optimization algorithms. Classes APPSEvalMgr and COLINApplication provide the function evaluation interface for APPSOptimizer and COLINNOptimizer, respectively.

- Parameter estimation: **LeastSq** provides a base class for NL2SOLLeastSq, a least-squares solver based on NL2SOL, SNLLLeastSq, a Gauss-Newton least-squares solver, and NLSSOLLeastSq, an SQP-based least-squares solver.

- Surrogate-based minimization (both optimization and nonlinear least squares): **SurrBasedMinimizer** provides a base class for SurrBasedLocalMinimizer, SurrBasedGlobalMinimizer, and EffGlobalMinimizer. The surrogate-based local and global methods employ a single iterator with any of the available Surrogate-Model capabilities (local, multipoint, or global data fits or hierarchical approximations) and perform a sequence of approximate optimizations, each involving build, optimize, and verify steps. The efficient global method, on the other hand, hard-wires a recursion involving Gaussian process surrogate models coupled with the DIRECT global optimizer to maximize an expected improvement function.

The Analyzer classes are grouped into:

- Uncertainty quantification: **NonD** provides a base class for non-deterministic methods in several categories:
  - Sampling: **NonDSampling** is further specialized with the NonDLHSSampling class for Latin hypercube and Monte Carlo sampling, and a number of other classes supporting incremental and adaptive sampling such as NonDAadaptImpSampling for multi-modal adaptive importance sampling.
  - Reliability Analysis: **NonDReliability** is further specialized with local and global methods (NonDLocalReliability and NonDGlobalReliability). NonDPOFDarts implements a computational geometry-based reliability method.
  - Stochastic Expansions: **NonDExpansion** includes specializations for generalized polynomial chaos (NonDPolynomialChaos) and stochastic collocation (NonDStochCollocation) and is supported by the NonDIntegration helper class, which supplies cubature, tensor-product quadrature and Smolyak sparse grid methods (NonDCubature, NonDQuadrature, and NonDSparseGrid).
  - Bayesian Calibration: **NonDCalibration** provides a base class for nondeterministic calibration methods with specialization to Bayesian calibration in NonDBayesCalibration, and specific implementations such as NonDUESOBayesCalibration.
  - **NonDInterval** provides a base class for epistemic interval-based UQ methods. Three interval analysis approaches are provided: LHS (NonDLhsInterval), efficient global optimization (NonDGlobalInterval), and local optimization (NonDLocalInterval). Each of these three has specializations for single interval and Dempster-Shafer Theory of Evidence approaches.

- Parameter studies and design of experiments: **PStudyDACE** provides a base class for ParamStudy, which provides capabilities for directed parameter space interrogation, PSUADEDesignCompExp, which provides access to the Morris One-At-a-Time (MOAT) method for parameter screening, and DDACEDesignCompExp and FSUDesignCompExp, which provide for parameter space exploration through design and analysis of computer experiments. NonDLHSSampling from the uncertainty quantification branch also supports design of experiments when in active all variables mode.

- Solution verification studies: **Verification** provides a base class for RichExtrapVerification (verification via Richardson extrapolation) and other solution verification methods in development.
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1.2.3 Models

Class hierarchy: Model.

The model classes are responsible for mapping variables into responses when an iterator makes a function evaluation request. There are several types of models, some supporting sub-iterators and sub-models for enabling layered and nested relationships. When sub-models are used, they may be of arbitrary type so that a variety of recursions are supported.

- SimulationModel: variables are mapped into responses using a simulation-based Interface object. No sub-iterators or sub-models are used.

- SurrogateModel: variables are mapped into responses using an approximation. The approximation is built and/or corrected using data from a sub-model (the truth model) and the data may be obtained using a sub-iterator (a design of experiments iterator). SurrogateModel has two derived classes: DataFitSurrModel for data fit surrogates and HierarchSurrModel for hierarchical models of varying fidelity. The relationship of the sub-iterators and sub-models is considered to be “layered” since they are not used as part of every response evaluation on the top level model, but rather used periodically in surrogate update and verification steps.

- NestedModel: variables are mapped into responses using a combination of an optional Interface and a sub-iterator/sub-model pair. The relationship of the sub-iterators and sub-models is considered to be “nested” since they are used to perform a complete iterative study as part of every response evaluation on the top level model.

- RecastModel: recasts the inputs and outputs of a sub-model for the purposes of variable transformations (e.g., variable scaling, transformations to standardized random variables) and problem reformulation (e.g., multi-objective optimization, response scaling, augmented Lagrangian merit functions, expected improvement).

1.2.4 Variables

Class hierarchy: Variables.

The Variables class hierarchy manages design, aleatory uncertain, epistemic uncertain, and state variable types for continuous, discrete integer, and discrete real domain types. This hierarchy is specialized according to how the domain types are managed:

- MixedVariables: domain type distinctions are retained, such that separate continuous, discrete integer, and discrete real domain types are managed. This is the default Variable perspective, and draws its name from “mixed continuous-discrete” optimization.

- RelaxedVariables: domain types are combined through relaxation of discrete constraints; i.e., continuous and discrete variables are merged into continuous arrays through relaxation of integrality (for discrete integer ranges) or set membership (for discrete integer or discrete real sets) requirements. The branch and bound minimizer is the only method using this approach at present.

Whereas domain types are defined based on the derived Variables class selection, the selection of active variable types is handled within each of these derived classes using variable views. These permit different algorithms to work on different subsets of variables. Data shared among Variables instances is stored in SharedVariablesData. For details on managing variables, see Working with Variable Containers and Views.

The Constraints hierarchy manages bound, linear, and nonlinear constraints and utilizes the same specializations for managing bounds on the variables (see MixedVarConstraints and RelaxedVarConstraints).
1.2. OVERVIEW OF DAKOTA

1.2.5 Interfaces

Class hierarchy: Interface.

Interfaces provide access to simulation codes or, conversely, approximations based on simulation code data. In the simulation case, an ApplicationInterface is used. ApplicationInterface is specialized according to the simulation invocation mechanism, for which the following nonintrusive approaches are supported:

- **SysCallApplicInterface**: the simulation is invoked using a system call (the C function `system()`). Asynchronous invocation utilizes a background system call. Utilizes the `CommandShell` utility.

- **ForkApplicInterface**: the simulation is invoked using a fork (the `fork/exec/wait` family of functions). Asynchronous invocation utilizes a nonblocking fork.

- **SpawnApplicInterface**: for Windows, fork is replaced by spawn. Asynchronous invocation utilizes a nonblocking spawn.

Fork and Spawn are inherited from ProcessHandleApplicInterface and System and ProcessHandle are inherited from ProcessApplicInterface. A semi-intrusive approach is also supported by:

- **DirectApplicInterface**: the simulation is linked into the Dakota executable and is invoked using a procedure call. Asynchronous invocations will utilize nonblocking threads (capability not yet available). Specializations of the direct interface are implemented in MatlabInterface, PythonInterface, ScilabInterface, and (for built-in testers) TestDriverInterface, while examples of plugin interfaces for library mode in serial and parallel, respectively, are included in SerialDirectApplicInterface and ParallelDirectApplicInterface

Scheduling of jobs for asynchronous local, message passing, and hybrid parallelism approaches is performed in the ApplicationInterface class, with job initiation and job capture specifics implemented in the derived classes.

In the approximation case, global, multipoint, or local data fit approximations to simulation code response data can be built and used as surrogates for the actual, expensive simulation. The interface class providing this capability is

- **ApproximationInterface**: builds an approximation using data from a truth model and then employs the approximation for mapping variables to responses. This class contains an array of Approximation objects, one per response function, which support a variety of approximation types using the different Approximation derived classes. These include SurfpackApproximation (provides kriging, MARS, moving least squares, neural network, polynomial regression, and radial basis functions), GaussProcApproximation (Gaussian process models), PecosApproximation (multivariate orthogonal and Lagrange interpolation polynomials from Pecos), TANA3Approximation (two-point adaptive nonlinearity approximation), and TaylorApproximation (local Taylor series).

which is an essential component within the DataFitSurrModel capability described above in Models.

1.2.6 Responses

Class: Response.

The Response class provides an abstract data representation of response functions and their first and second derivatives (gradient vectors and Hessian matrices). These response functions can be interpreted as objective functions and constraints (optimization data set), residual functions and constraints (least squares data set), or generic response functions (uncertainty quantification data set). This class is not currently part of a class hierarchy, since the abstraction has been sufficiently general and has not required specialization.
CHAPTER 1. DAKOTA DEVELOPERS MANUAL

1.3 Services

A variety of services and utilities are used in Dakota for parallel computing, failure capturing, restart, graphics, etc. An overview of the classes and member functions involved in performing these services is included here.

- **Multilevel parallel computing**: Dakota supports multiple levels of nested parallelism. A meta-iterator can manage concurrent iterators, each of which manages concurrent function evaluations, each of which manages concurrent analyses executing on multiple processors. Partitioning of these levels with MPI communicators is managed in ParallelLibrary and scheduling routines for the levels are part of IteratorScheduler, ApplicationInterface, and ForkApplicInterface.

- **Option management**: Global options controlling behavior are managed in ProgramOptions, with the help of command-line option parsing in CommandLineHandler.

- **Parsing**: Dakota employs NIDR (New Input Deck Reader) via Dakota::ProblemDescDB::parse inputs to parse user input files. NIDR uses the keyword handlers in the NIDRProblemDescDB derived class to populate data within the ProblemDescDB base class, which maintains a DataEnvironment specification and lists of DataMethod, DataModel, DataVariables, DataInterface, and DataResponses specifications. Procedures for modifying the parsing subsystem are described in Instructions for Modifying Dakota’s Input Specification.

- **Failure capturing**: Simulation failures can be trapped and managed using exception handling in ApplicationInterface and its derived classes.

- **Restart**: Dakota maintains a record of all function evaluations both in memory (for capturing any duplication) and on the file system (for restarting runs). Restart options are managed through ProgramOptions (with the help of CommandLineHandler); file management in OutputManager; and restart file insertions occur in ApplicationInterface. The dakota_restart_util executable, built from restart_util.cpp, provides a variety of services for interrogating, converting, repairing, concatenating, and post-processing restart files.

- **Memory management**: Dakota employs the techniques of reference counting and representation sharing through the use of letter-envelope and handle-body idioms (Coplien, “Advanced C++”). The former idiom provides for memory efficiency and enhanced polymorphism in the following class hierarchies: Environment, Iterator, Model, Variables, Constraints, Interface, ProblemDescDB, and Approximation. The latter idiom provides for memory efficiency in data-intensive classes which do not involve a class hierarchy. The Response and parser data (DataEnvironment, DataMethod, DataModel, DataVariables, DataInterface, and DataResponses) classes use this idiom. When managing reference-counted data containers (e.g., Variables or Response objects), it is important to properly manage shallow and deep copies, to allow for both efficiency and data independence as needed in a particular context.

- **Graphics and Output**: Dakota provides 2D iteration history graphics using Motif widgets. Graphics data can also be cataloged in a tabular data file for post-processing with 3rd party tools such as Matlab, Tecplot, etc. These capabilities are encapsulated within the Graphics class. An experimental results database is implemented in ResultsManager and ResultsDBAny. Options for controlling output and facilities for managing it are in OutputManager.

1.4 Development Practices and Guidance

The following links provide guidance for core software components or specific development activities:

- **Coding Style Guidelines and Conventions** - coding practices used by the Dakota development team.
1.5. ADDITIONAL RESOURCES

- Instructions for Modifying Dakota’s Input Specification - how to interact with NIDR and the associated Dakota classes.
- Interfacing with Dakota as a Library - embed Dakota as a service within your application.
- Understanding Iterator Flow - explanation of the full granularity of steps in Iterator execution.
- Performing Function Evaluations - an overview of the classes and member functions involved in performing function evaluations synchronously or asynchronously.
- Working with Variable Containers and Views - discussion of data storage for variables and explanation of active and inactive views of this data.

1.5 Additional Resources

Additional development resources include:

- The Dakota Developer Portal linked from [http://dakota.sandia.gov/content/developer-portal/](http://dakota.sandia.gov/content/developer-portal/) includes information on getting started as a developer and links to project management resources.
- Project web pages are maintained at [http://dakota.sandia.gov/](http://dakota.sandia.gov/) including links to frequently asked questions, documentation, publications, mailing lists, and other resources.
Chapter 2

Coding Style Guidelines and Conventions

2.1 Introduction

Common code development practices can be extremely useful in multiple developer environments. Particular styles for code components lead to improved readability of the code and can provide important visual cues to other developers. Much of this recommended practices document is borrowed from the CUBIT mesh generation project, which in turn borrows its recommended practices from other projects, yielding some consistency across Sandia projects. While not strict requirements, these guidelines suggest a best-practices starting point for coding in Dakota.

2.2 C++/c Style Guidelines

Style guidelines involve the ability to discern at a glance the type and scope of a variable or function.

2.2.1 Class and variable styles

Class names should be composed of two or more descriptive words, with the first character of each word capitalized, e.g.:

```cpp
class ClassName;
```

Class member variables should be composed of two or more descriptive words, with the first character of the second and succeeding words capitalized, e.g.:

```cpp
double classMemberVariable;
```

Temporary (i.e. local) variables are lower case, with underscores separating words in a multiple word temporary variable, e.g.:

```cpp
int temporary_variable;
```

Constants (i.e. parameters) and enumeration values are upper case, with underscores separating words, e.g.:

```cpp
const double CONSTANT_VALUE;
```
CHAPTER 2. CODING STYLE GUIDELINES AND CONVENTIONS

2.2.2 Function styles

Function names are lower case, with underscores separating words, e.g.:

```c
int function_name();
```

There is no need to distinguish between member and non-member functions by style, as this distinction is usually clear by context. This style convention allows member function names which set and return the value of a similarly-named private member variable, e.g.:

```c
int memberVariable;
void member_variable(int a) { // set
  memberVariable = a;
}
int member_variable() const { // get
  return memberVariable;
}
```

In cases where the data to be set or returned is more than a few bytes, it is highly desirable to employ const references to avoid unnecessary copying, e.g.:

```c
void continuous_variables(const RealVector& c_vars) { // set
  continuousVariables = c_vars;
} const RealVector& continuous_variables() const { // get
  return continuousVariables;
}
```

Note that it is not necessary to always accept the returned data as a const reference. If it is desired to be able change this data, then accepting the result as a new variable will generate a copy, e.g.:

```c
const RealVector& c_vars = model.continuous_variables(); // reference to continuousVariables cannot be changed
RealVector c_vars = model.continuous_variables(); // local copy of continuousVariables can be changed
```

2.2.3 Miscellaneous

Appearance of typedefs to redefine or alias basic types is isolated to a few header files (data_types.h, template_defs.h), so that issues like program precision can be changed by changing a few lines of typedefs rather than many lines of code, e.g.:

```c
typedef double Real;
```

_Xemacs_ is the preferred source code editor, as it has C++ modes for enhancing readability through color (turn on "Syntax highlighting"). Other helpful features include "Paren highlighting" for matching parentheses and the "New Frame" utility to have more than one window operating on the same set of files (note that this is still the same edit session, so all windows are synchronized with each other). Window width should be set to 80 internal columns, which can be accomplished by manual resizing, or preferably, using the following alias in your shell resource file (e.g., .cshrc):

```c
alias xemacs "xemacs -g 81x63"
```

where an external width of 81 gives 80 columns internal to the window and the desired height of the window will vary depending on monitor size. This window width imposes a coding standard since you should avoid line wrapping by continuing anything over 80 columns onto the next line.

Indenting increments are 2 spaces per indent and comments are aligned with the code they describe, e.g.:
2.3. FILE NAMING CONVENTIONS

Also, the continuation of a long command is indented 2 spaces, e.g.:

```cpp
const String& iterator_scheduling = problem_db.get_string("strategy.iterator.scheduling");
```

and similar lines are aligned for readability, e.g.:

```cpp
cout << "Numerical gradients using " << finiteDiffStepSize*100. << "\%" << finiteDiffType << " differences to be calculated by the " << methodSource << " finite difference routine." << endl;
```

Lastly, #ifdef’s are not indented (to make use of syntax highlighting in xemacs).

2.3 File Naming Conventions

In addition to the style outlined above, the following file naming conventions have been established for the Dakota project.

File names for C++ classes should, in general, use the same name as the class defined by the file. Exceptions include:

- with the introduction of the Dakota namespace, base classes which previously utilized prepended Dakota identifiers can now safely omit the identifiers. However, since file names do not have namespace protection from name collisions, they retain the prepended Dakota identifier. For example, a class previously named DakotaModel which resided in DakotaModel.cpp/hpp, is now Dakota::Model (class Model in namespace Dakota) residing in the same filenames. The retention of the previous filenames reduces the possibility of multiple instances of a Model.hpp causing problems. Derived classes (e.g., NestedModel) do not require a prepended Dakota identifier for either the class or file names.

- in a few cases, it is convenient to maintain several closely related classes in a single file, in which case the file name may reflect the top level or some generalization of the set of classes (e.g., DakotaResponse.[CH] files contain Dakota::Response and Dakota::ResponseRep classes, and DakotaBinStream.[CH] files contain the Dakota::BiStream and Dakota::BoStream classes).

The type of file is determined by one of the four file name extensions listed below:

- **.hpp** A class header file ends in the suffix .hpp. The header file provides the class declaration. This file does not contain code for implementing the methods, except for the case of inline functions. Inline functions are to be placed at the bottom of the file with the keyword inline preceding the function name.

- **.cpp** A class implementation file ends in the suffix .cpp. An implementation file contains the definitions of the members of the class.
• .h A header file ends in the suffix .h. The header file contains information usually associated with procedures. Defined constants, data structures and function prototypes are typical elements of this file.

• .c A procedure file ends in the suffix .c. The procedure file contains the actual procedures.

2.4 Class Documentation Conventions

Class documentation uses the doxygen tool available from http://www.doxygen.org and employs the J-AVA-doc comment style. Brief comments appear in header files next to the attribute or function declaration. Detailed descriptions for functions should appear alongside their implementations (i.e., in the .cpp files for non-inlined, or in the headers next to the function definition for inlined). Detailed comments for a class or a class attribute must go in the header file as this is the only option.

NOTE: Previous class documentation utilities (class2frame and class2html) used the ”//” comment style and comment blocks such as this:

```c
//-- Class: Model
//-- Description: The model to be iterated by the Iterator.
//-- Contains Variables, Interface, and Response objects.
//-- Owner: Mike Eldred
```

These tools are no longer used, so remaining comment blocks of this type are informational only and will not appear in the documentation generated by doxygen.

2.5 CMake Style Guidelines

Dakota conventions for CMake files, such as CMakeLists.txt, FooConfig.cmake, etc., follow. Our goal is ease of reading, maintenance, and support, similar to the C++ code itself. Current CMake versions and build hints are maintained at the Developer Portal http://dakota.sandia.gov/developer/.

2.5.1 CMake Code Formatting

• Indentation is 2 spaces, consistent with Dakota C++ style.

• Lines should be kept to less than 80 chars per line where possible.

• Wrapped lines may be indented two spaces or aligned with prior lines.

• For ease of viewing and correctness checking in Emacs, a customization file is available: http://www.-cmake.org/CMakeDocs/cmake-mode.el

2.5.2 CMake Variable Naming Conventions

These variable naming conventions are especially important for those that ultimately become preprocessor defines and affect compilation of source files.

• Classic/core elements of the CMake language are set in lower_case, e.g., option, set, if, find_library.

• Static arguments to CMake functions and macros are set in UPPER_CASE, e.g. REQUIRED, NO_MODULE, QUIET.

• Minimize ”global” variables, i.e., don’t use 2 variables with the same meaning when one will do the job.
2.5. **CMAKE STYLE GUIDELINES**

- Feature toggling: when possible, use the "HAVE_<pkg/feature>" convention already in use by many CMake-enabled TPLs, e.g.,

  ```
  $ grep HAVE_SYSTEM Dakota/src/CMakeLists.txt
  check_function_exists(system HAVE_SYSTEM)
  if(HAVE_SYSTEM)
    add_definitions("-DHAVE_SYSTEM")
  endif(HAVE_SYSTEM)
  $ grep HAVE_CONMIN Dakota/src/CMakeLists.txt Dakota/packages/CMakeLists.txt
  Dakota/src/CMakeLists.txt:if(HAVE_CONMIN)
  Dakota/src/CMakeLists.txt:endif(HAVE_CONMIN)
  Dakota/packages/CMakeLists.txt:option(HAVE_CONMIN "Build the CONMIN package." ON)
  Dakota/packages/CMakeLists.txt:endif(HAVE_CONMIN)
  ```

- When a variable/preprocessor macro could result in name clashes beyond Dakota scope, e.g., for library-mode users, consider prefixing the "HAVE_<pkg>" name with DAKOTA_, e.g. DAKOTA_HAVE_MPI. Currently, MPI is the only use case for such a variable in Dakota, but many examples can be found in the CMake Modules source, e.g.

  ```
  grep _HAVE_ <cmake_prefix_dir>/share/cmake-2.8/Modules/*
  ```
Chapter 3

Instructions for Modifying Dakota’s Input Specification

To modify Dakota’s input specification (for maintenance or addition of new input syntax), specification maintenance mode must be enabled at Dakota configure time with the `–ENABLE_SPEC_MAINT` option, e.g.,

```
./cmake –ENABLE_SPEC_MAINT:BOOL=ON ..
```

This will enable regeneration of NIDR and Dakota components which must be updated following a spec change.

3.1 XML Input Specification

The authoritative source for valid Dakota input grammar is `dakota/src/dakota.xml`. The schema defining valid content for this XML file is in `dakota/src/dakota.xsd`. NIDR remains Dakota’s user input file parser, so `dakota.xml` is translated to `dakota/src/dakota.input.nspec` during the Dakota build process. To update the XML input definition:

- Make sure `ENABLE_SPEC_MAINT` is enabled in your build and necessary Java development tools are installed (see below).
- Edit the XML spec in `dakota.xml`.
- Perform a make in `dakota.build/src` which will regenerate `dakota.source/src/dakota.input.nspec` and related file.
- Review that any changes induced in the `dakota.input.nspec` file are as expected.
- Proceed with verifying code changes and making downstream parse handler changes as normal (described below).
- Commit the modified `dakota.xml`, `dakota.input.nspec`, and other files generated to `dakota-source/src` along with your other code changes.

3.1.1 XML Build Requirements

Editing the XML and then compiling Dakota requires
• Java Development Kit (JDK) providing the Java compiler javac. Java 6 (version 1.6) or newer should work, with Java 8 recommended. Can satisfy on RHEL6 with RPM packages `java-1.8.0-openjdk-devel` and `java-1.8.0-openjdk`. This is needed to build the Java-based XML to NIDR translator. If this becomes too burdensome, we can check in the generated `xml2nidr.jar` file.

### 3.1.2 XML Editing Tools

The following tools will make editing `dakota.input.xml` easier.

- **Recommended:** Eclipse Web Tools Platform. Includes both graphical and text editors.
  1. Download Eclipse Standard (Classic)
  2. Configure proxy if needed, setting to manual: Window > Preferences > General > Network Connection > Proxy
  3. Install Web Tools Platform
     - Help > Install New Software
     - Work With: Kepler - [http://download.eclipse.org/releases/kepler](http://download.eclipse.org/releases/kepler)
     - Search "Eclipse X" and install two packages under Web, XML, Java
       * Eclipse XML Editors and Tools
       * Eclipse XSL Developer Tools
     - Optionally install C/C++ Development Tools
  4. Optional: add Subclipse for subversion (Subversive is the other major competing tool and I don’t think requires JavaHL) Help > Install New Software Work With: [http://subclipse.tigris.org/update_1.6.x](http://subclipse.tigris.org/update_1.6.x) Install Subclipse On Linux: `yum install subversion-javahl.x86_64`
  5. Alternately install Eclipse for Java or Eclipse Java EE development which includes webtools, then optionally add subclipse and C/C++ dev

- **Alternate:** Emacs or your usual editor. For example, Emacs supports an Nxml mode. You can tell it where to find the schema, edit XML, and have it perform validation against the schema. See help at [http://www.gnu.org/software/emacs/manual/html_mono/nxml-mode.html](http://www.gnu.org/software/emacs/manual/html_mono/nxml-mode.html)

- **Other Suggested Alternates:** XMLSpy, DreamWeaver, XML Copy Editor

### 3.1.3 XML Features (with map to NIDR)

Out of necessity, Dakota XML `dakota.xml` closely mirrors `dakota.input.nspec`. Valid Dakota input grammar is constrained by `dakota.xml`, an XML document which must validate against `dakota.xsd`. The top-level element of interest is `<input>`, which is comprised of a sequence of content elements (keywords, alternates, etc.), which may themselves contain additional child content elements. The key content types are:

- **Keyword** (`<keyword>`): specified with the `<keyword>` element whose definition is given by `keyword-Type` in `dakota.xsd`. The required attributes are:
  - **name**: The keyword name (lower case with underscores) as it will be given in user input; must follow same uniqueness rules are historical NIDR. User input is allowed in mixed case, but the XML must use lower case names.

  Since the NIDR parser allows keyword abbreviation, you **must** not add a keyword that could be mis-interpreted as an abbreviation for a different keyword within the same top-level keyword, such as
“environment” and “method”. For example, adding the keyword “expansion” within the method specification would be a mistake if the keyword “expansion_factor” already was being used in this block.

The NIDR input is somewhat order-dependent, allowing the same keyword to be reused multiple times in the specification. This often happens with aliases, such as lower_bounds, upper_bounds and initial_point. Ambiguities are resolved by attaching a keyword to the most recently seen context in which it could appear, if such exists, or to the first relevant context that subsequently comes along in the input file.

- **code**: The verbatim NIDR handler to be invoked when this keyword parsed. In NIDR this was specified with {N_macro(...)}.

Optional/useful parser-related elements/attributes in order of importance are:

- **param sub-element**: Parameters and data types: A keyword may have an associated parameter element with a specified data type: `<param type="PARAMTYPE" />`. NIDR data types remain the same (INTEGER, REAL, STRING and LISTS thereof, but new data types INPUT_FILE and OUTPUT_FILE add convenience for the GUI, mapping to STRING for NIDR purposes. Parameters can also include attributes constraint, in_taglist, or taglist, which are used to help validate the user-specified parameter value. For example `constraint >= 0 LEN normal uncertain`

- **alias sub-element**: Historical aliases for this keyword (can appear multiple times). Alias has a single attribute name which must be lower case with underscores.

- **id**: Unique ID for the keyword, usually name with an integer appended, but not currently used/enforced.

- **minOccurs**: Minimum occurrences of the keyword in current context (set to 1 for required, 0 for optional)

- **maxOccurs**: Maximum occurrences of the keyword in current context (for example environment may appear at most once)

And optional/useful GUI-related attributes are:

- **help**: (Don’t add this attribute the new keywords!) A pointer to the corresponding reference manual section (deprecated as not needed with new reference manual format which mirrors keyword hierarchy).

- **label**: a short, friendly label string for the keyword in the GUI. Format these like titles, e.g., "Initial Point for Search".

- **group**: Category or group for this keyword, e.g., optimization vs. parameter study if they are to be groups for GUI purposes

- **Alternation ( <oneOf> )**: Alternation of groups of content is done with the element `<oneOf>` which indicates that its immediate children are alternates. In NIDR this was done with the pipe symbol: OptionA | OptionB. oneOf allows the label attribute and its use is recommended.

- **Required Group ( <required> )**: A required group can be specified by enclosing the contents in the `<required>` element. In NIDR this was done by enclosing the content in parentheses: ( required group... )

- **Optional Group ( <optional> )**: An optional group can be specified by enclosing the contents in the `<optional>` element. In NIDR this was done by enclosing the content in brackets: [ optional group... ]
3.2 Rebuild Generated Files

When configured with `-DENABLE_SPEC_MAINT`, performing a make in `dakota.build/src` will regenerate all files which derive from `dakota.xml`, include `dakota.input.nspec`, `NIDR_keywds.hpp`, and `dakota.input-` summary. If you commit changes to a source repository, be sure to commit any automatically generated files in addition to any modified in the following steps. It is not strictly necessary to run make at this point in the sequence, and in fact may generate errors if necessary handlers aren’t yet available.

Warning

Please do not manually modify generated files!

3.3 Update Parser Source NIDRProblemDescDB.cpp

Many keywords have data associated with them: an integer, a floating-point number, a string, or arrays of such entities. Data requirements are specified in `dakota.input.nspec` by the tokens `INTEGER`, `REAL`, `STRING`, `INTEGERLIST`, `REALLIST`, `STRINGLIST`. (Some keywords have no associated data and hence no such token.) After each keyword and data token, the `dakota.input.nspec` file specifies functions that the NIDR parser should call to record the appearance of the keyword and deal with any associated data. The general form of this specification is

```
{ startfcn, startdata, stopfcn, stopdata }
```

i.e., a brace-enclosed list of one to four functions and data pointers, with trailing entities taken to be zero if not present; zero for a function means no function will be called. The startfcn must deal with any associated data. Otherwise, the distinction between startfcn and stopfcn is relevant only to keywords that begin a group of keywords (enclosed in parentheses or square brackets). The startfcn is called before other entities in the group are processed, and the stop function is called after they are processed. Top-level keywords often have both startfcn and stopfcn; stopfcn is uncommon but possible for lower-level keywords. The startdata and (if needed) stopdata values are usually pointers to little structures that provide keyword-specific details to generic functions for startfcn and stopfcn. Some keywords that begin groups (such as "approx_problem" within the top-level "environment" keyword) have no need of either a startfcn or a stopfcn; this is indicated by "{0}".

Most of the things within braces in `dakota.input.nspec` are invocations of macros defined in `dakota-source/src/NIDRProblemDescDB.cpp`. The macros simplify writing `dakota.input.nspec` and make it more readable. Most macro invocations refer to little structures defined in NIDRProblemDescDB.cpp, usually with the help of other macros, some of which have different definitions in different parts of NIDRProblemDescDB.cpp. When adding a keyword to `dakota.input.nspec`, you may need to add a structure definition or even introduce a new data type. NIDRProblemDescDB.cpp has sections corresponding to each top-level keyword. The top-level keywords are in alphabetical order, and most entities in the section for a top-level keyword are also in alphabetical order. While not required, it is probably good practice to maintain this structure, as it makes things easier to find.

Any integer, real, or string data associated with a keyword are provided to the keyword’s startfcn, whose second argument is a pointer to a `Values` structure, defined in header file `nidr.h`.

**Example 1:** if you added the specification:

```
[method_setting REAL {method_setting_start, &method_setting_details}]
```

you would provide a function

```c++
void NIDRProblemDescDB::
method_setting_start(const char *keyname, Values *val, void **g, void *v)
{
...}
```

in NIDRProblemDescDB.cpp. In this example, argument `&method_setting_details` would be passed as `v`, `val->n` (the number of values) would be 1 and `*val->r` would be the REAL value given for the method-setting keyword. The `method_setting_start` function would suitably store this value with the help of `method_setting_details`. 
3.4. UPDATE CORRESPONDING DATA CLASSES

For some top-level keywords, \( g \) (the third argument to the startfcn and stopfcn) provides access to a relevant context. For example, method_start (the startfcn for the top-level method keyword) executes

```cpp
DataMethod *dm = new DataMethod;
g = (void*)dm;
```
(and supplies a couple of default values to \( dm \)). The start functions for lower-level keywords within the method keyword get access to \( dm \) through their \( g \) arguments. Here is an example:

```cpp
void NIDRProblemDescDB::method_str(const char *keyname, Values *val, void **g, void *v) {
    (*(DataMethod**)g)->**(String DataMethod::*v) = *val->s;
}
```

In this example, \( v \) points to a pointer-to-member, and an assignment is made to one of the components of the DataMethod object pointed to by \( *g \). The corresponding stopfcn for the top-level method keyword is

```cpp
void NIDRProblemDescDB::method_stop(const char *keyname, Values *val, void **g, void *v) {
    DataMethod *p = *(DataMethod**)g;
pDDBInstance->dataMethodList.insert(*p);
delete p;
}
```

which copies the now populated DataMethod object to the right place and cleans up.

**Example 2:** if you added the specification

```latex
[method_setting REALLIST \{(N_mdm(RealL,methodCoeffs)\]
```
then method_RealL (defined in NIDRProblemDescDB.cpp) would be called as the startfcn, and methodCoeffs would be the name of a (currently nonexistent) component of DataMethod. The N_mdm macro is defined in NIDRProblemDescDB.cpp; among other things, it turns RealL into NIDRProblemDescDB::method_RealL. This function is used to process lists of REAL values for several keywords. By looking at the source, you can see that the list values are \( val->r[i] \) for \( 0 <= i < val->n. \)

### 3.4 Update Corresponding Data Classes

The Data classes (DataEnvironment, DataMethod, DataModel, DataVariables, DataInterface, and DataResponses) store the parsed user input data. In this step, we extend the Data class definitions to include any new attributes referred to in dakota.xml or NIDRProblemDescDB

#### 3.4.1 Update the Data Class Header File

Add a new attribute to the public data for each of the new specifications. Follow the style guide for class attribute naming conventions (or mimic the existing code).

#### 3.4.2 Update the .cpp File

Define defaults for the new attributes in the constructor initialization list (if not a container with a sensible default constructor) in same order as they appear in the header. Add the new attributes to the write(MPIPackBuffer&), read(MPIUnpackBuffer&), and write(ostream&) functions, paying careful attention to the use of a consistent ordering.
CHAPTER 3. INSTRUCTIONS FOR MODIFYING DAKOTA'S INPUT SPECIFICATION

3.5 Update Database Source ProblemDescDB.cpp

3.5.1 Augment/update get_<data_type>() Functions

The next update step involves extending the database retrieval functions in dakota.source/src/ProblemDescDB.cpp. These retrieval functions accept an identifier string and return a database attribute of a particular type, e.g., a RealVector:

```cpp
const RealVector& get_rv(const String& entry_name);
```

The implementation of each of these functions contains tables of possible entry_name values and associated pointer-to-member values. There is one table for each relevant top-level keyword, with the top-level keyword omitted from the names in the table. Since binary search is used to look for names in these tables, each table must be kept in alphabetical order of its entry names. For example,

```cpp
... else if ((L = Begins(entry_name, "model."))) {
    if (dbRep->methodDBLocked)
        Locked_db();
    #define P &DataModelRep::
    static KW<RealVector, DataModelRep> RVdmo[] = {
        // must be sorted
        {"nested.primary_response_mapping", P primaryRespCoeffs},
        {"nested.secondary_response_mapping", P secondaryRespCoeffs},
        {"surrogate.kriging_conmin_seed", P krigingConminSeed},
        {"surrogate.kriging_correlations", P krigingCorrelations},
        {"surrogate.kriging_max_correlations", P krigingMaxCorrelations},
        {"surrogate.kriging_min_correlations", P krigingMinCorrelations}    
    };
    #undef P
    KW<RealVector, DataModelRep>* kw;
    if ((kw = (KW<RealVector, DataModelRep>*)Binsearch(RVdmo, L)))
        return dbRep->dataModelIter->dataModelRep->*kw->p;
}
```

is the "model" portion of ProblemDescDB::get_rv(). Based on entry_name, it returns the relevant attribute from a DataModel object. Since there may be multiple model specifications, the dataModelList list iterator identifies which node in the list of DataModel objects is used. In particular, dataModelList contains a list of all of the data_model objects, one for each time a top-level model keyword was seen by the parser. The particular model object used for the data retrieval is managed by dataModelIter, which is set in a set_db-list_nodes() operation that will not be described here.

There may be multiple DataMethod, DataModel, DataVariables, DataInterface, and/or DataResponses objects. However, only one specification is currently allowed so a list of DataEnvironment objects is not needed. Rather, ProblemDescDB::environmentSpec is the lone DataEnvironment object.

To augment the get_<data_type>() functions, add table entries with new identifier strings and pointer-to-member values that address the appropriate data attributes from the Data class object. The style for the identifier strings is a top-down hierarchical description, with specification levels separated by periods and words separated with underscores, e.g., "keyword.group_specification.individual_specification". Use the dbRep->listIter->attribute syntax for variables, interface, responses, and method specifications. For example, the method_setting example attribute would be added to get_rv() as:

```cpp
{"method_name.method_setting", P methodSetting},
```

inserted at the beginning of the RVdmo array shown above (since the name in the existing first entry, i.e., "nested.primary_response_mapping", comes alphabetically after "method_name.method_setting").
3.6 Use get_<data_type>() Functions

At this point, the new specifications have been mapped through all of the database classes. The only remaining step is to retrieve the new data within the constructors of the classes that need it. This is done by invoking the get_<data_type>() function on the ProblemDescDB object using the identifier string you selected in Augment/update get_<data_type>() Functions. For example:

```cpp
const String& interface_type = problem_db.get_string("interface.type");
```

passes the "interface.type" identifier string to the ProblemDescDB::get_string() retrieval function, which returns the desired attribute from the active DataInterface object.

Warning

Use of the get_<data_type>() functions is restricted to class constructors, since only in class constructors are the data list iterators (i.e., dataMethodIter, dataModelIter, dataVariablesIter, dataInterfaceIter, and dataResponsesIter) guaranteed to be set correctly. Outside of the constructors, the database list nodes will correspond to the last set operation, and may not return data from the desired list node.

3.7 Update the Documentation

Doxygen comments should be added to the Data class headers for the new attributes, and the reference manual sections describing the portions of dakota.xml that have been modified should be updated by updating files in dakota.source/docs/KeywordMetaData/.dakota.xml, together with these metadata files generates the reference manual and GUI context-aware help documentation.
Chapter 4

Understanding Iterator Flow

This page explains the various phases comprising Iterator::run_iterator(). Prior to Iterator construction, when command-line options are parsed, Boolean run mode flags corresponding to PRERUN, RUN, and POSTRUN are set in ParallelLibrary. If the user didn’t specify any specific run modes, the default is for all three to be true (all phases will execute).

Iterator is constructed.

When called, run_iterator() sequences:

- **initialize_run():** unconditionally called, virtual. Performs common initialization such as allocating workspaces, setting communicators and evaluation counts. When re-implementing this virtual, a derived class must call its nearest parent’s initialize_run(), typically before performing its own implementation steps.

- **Not implemented: pre-run input**

- IF PRERUN, invoke pre_run(): virtual function; default no-op. Purpose: derived classes should implement pre_run() if they are able to generate all parameter sets (variables) at once, separate from run(). Derived implementations should call their nearest parent’s pre_run(), typically before performing their own steps.

- **Not implemented: run input**

- IF RUN, invoke virtual function run(). Purpose: at a minimum, evaluate parameter sets through computing responses; for iterators without pre/post capability, their entire implementation is in run() and this is a reasonable default for new Iterators.

- **Not implemented: run output**

- IF POSTRUN, invoke post_input(): virtual function, default only print helpful message on mode. Purpose: derived iterators supporting post-run input from file must implement to read file and populate variables/responses (and possibly best points) appropriately. Implementations must check if the user requested file input.

- **Not implemented: post-run output**
• `finalize_run()`: unconditionally called, virtual. Purpose: free workspaces. Default base class behavior is no-op, however, derived implementations should call their nearest parent’s `finalize_run` after performing their specialized portions.

`Iterator` is destructed.
Chapter 5

Interfacing with Dakota as a Library

5.1 Introduction

Tightly integrating or linking Dakota into another application can improve user experience by delivering a more unified, inter-operable software tool for optimization and UQ analyses, improving performance by eliminating file system-based interfaces, and reducing challenges with parallel computing inter-operation. This benefit has been realized within several Sandia and external simulation applications. This section describes how to link Dakota into another C++ application.

Dakota has two primary application programming interfaces (APIs). The LibraryEnvironment class facilitates use of Dakota as an algorithm service library within another application. In this case, the simulation application is providing a "front end" for Dakota. The second API, provided by the DirectApplicInterface class, provides an interface for Dakota to call the simulation code directly to perform function evaluations in core. This permits the simulation to be the "back end" for Dakota. The most complete library integration of Dakota would use both in combination, with the overall simulation framework providing both the front end and back end for Dakota, creating a sandwich, as loosely depicted here:

```
[------------
| Application
| |
| { ----- |
| { Dakota (LibraryEnvironment)
| |
| { { Function evaluation callback to Application (via DirectApplicInterface)
| { { |
| {-------/ |
| { |
| { |
| { ----- |
|------------
```

Attention

Dakota may be integrated as a library in other software applications subject to the terms of the GNU Lesser General Public License (LGPL). Refer to http://www.gnu.org/licenses/lgpl.html or the LICENSE file included with Dakota.

When Dakota is compiled and installed, the relevant library API headers are installed to CMAKE_INSTALL_PREFIX/include and the runtime libraries primarily to CMAKE_INSTALL_PREFIX/lib/ (on some platforms,
to CMAKE_INSTALL_PREFIX/bin/. The core C/C++ code is in the library dakota_src, while Fortran code lives in the dakota_src_fortran library. Information on using the API in Dakota headers is included throughout this section, while considerations for configuring and linking against Dakota and its various required and optional third–party libraries are emphasized in the section Linking against the Dakota library.

Steps involved in integrating Dakota into another application typically include:

1. Writing C++ code for your application to instantiate, configure, and execute Dakota’s LibraryEnvironment (“front end”); see Basic Dakota library instantiation and Configuring Dakota operation.

2. Writing C++ code for Dakota to call a function in your application to perform function evaluations (“back end”); see Creating a simulator plugin interface.

3. Compiling Dakota and linking into your application (Linking against the Dakota library).

Several source code examples demonstrate Dakota library interfaces. The classes SIM::SerialDirectApplicInterface and SIM::ParallelDirectApplicInterface demonstrate serial and parallel simulation function evaluation plug-ins. The file library_mode.cpp includes a main program that exercises Dakota libraries in serial and parallel modes with these mock simulator programs, with various ways of configuring Dakota problem definition and operation. Finally, library_split.cpp demonstrates running Dakota as a library modular on an MPI sub-communicator.

5.2 Basic Dakota library instantiation

The function run_dakota_parse() in library_mode.cpp demonstrates the basic use of Dakota library objects as one would in another main application that embeds Dakota. In this example, Dakota is configured based on a typical user-provided text-based Dakota input file (the same that would be provided at the command line with dakota-optimization.in) and a function evaluator derived from a DirectApplicInterface is plugged into the Dakota library environment.

First, an object of type ProgramOptions which manages top-level Dakota settings is instantiated and configured to specify the name of the Dakota user input file. Additional options for output and error redirection, restart operation, and more may be set via ProgramOptions. See its class documentation for details.

```cpp
string dakota_input_file = "dakota_optimization.in";
Dakota::ProgramOptions opts;
opts.input_file(dakota_input_file);
```

Next, a LibraryEnvironment is created, passing the desired settings from opts:

```cpp
Dakota::LibraryEnvironment env(opts);
```

This standard constructor will parse the specified input and create Dakota objects. It assumes many default settings, including that the parent application initialized MPI if running in parallel mode. (In this case, Dakota will detect whether MPI was initialized and not call MPI_Init or MPI_Finalize.) For more advanced use cases described below, alternate constructors allow constructing based on MPI communicators, with delayed finalization, and with Dakota database update function callbacks. Then the application’s function evaluator implementing Dakota’s DirectApplicInterface is plugged in with a convenience function serial_interface_plugin() or parallel_interface_plugin(). Finally, the Dakota analysis is run by calling

```cpp
env.execute();
```

The next two sections offer additional details on (1) alternative and supplementary ways to configure Dakota’s operation (Configuring Dakota operation) and (2) how to specialize Dakota’s DirectApplicInterface to provide a function evaluator plugin to Dakota (Creating a simulator plugin interface).
Remarks

After LibraryEnvironment construction, all MPI communicator partitioning has been performed and the ParallelLibrary instance may be interrogated for parallel configuration data. For example, the lowest level communicators in Dakota’s multilevel parallel partitioning are the analysis communicators, which can be retrieved using:

```cpp
// retrieve the set of analysis communicators for simulation initialization:
// one analysis comm per ParallelConfiguration (PC), one PC per Model.
Array<MPI_Comm> analysis_comms = parallel_lib.analysis_intra_communicators();
```

These communicators can then be used for initializing parallel simulation instances when registering the plugin interface, where the number of MPI communicators in the array corresponds to one communicator per ParallelConfiguration instance. This is demonstrated below in Derivation.

5.3 Configuring Dakota operation

This section describes several alternate ways to initially set and later manipulate Dakota’s configuration, including alternatives to using a text-based input file. The algorithm configuration for a particular Dakota analysis run is managed in its ProblemDescDB, which can be populated via an input file, string literal, or C++ API, and later modified through Dakota’s C++ API. All Dakota objects then draw information from this database upon instantiation.

5.3.1 Input data parsing

The simplest way for an application to configure a Dakota analysis problem is to use Dakota’s normal input parsing system to populate its problem database (ProblemDescDB). This is done by providing standard Dakota input file syntax through the library interface, via either a file name or string literal. An advantage is that native Dakota syntax can be used, but disadvantages include the requirement for an additional input file beyond those already required by the parent application and that application users also need to know Dakota syntax.

The two ways to configure Dakota via input parsing are shown near the beginning of run_dakota_mixed() in library_mode.cpp. Here the ProgramOptions are set to either parse from a named file:

```cpp
Dakota::ProgramOptions opts;
opts.input_file(dakota_input_file);
```

or from a string literal provided by the wrapping application:

```cpp
string serial_input = "& Dakota input file ...";
opts.input_string(serial_input);
```

This library approach is coarse-grained in that input is parsed, objects constructed, and the environment is immediately ready to run. The next approaches are more modular.

5.3.2 Problem database insertion

A second approach to configuring Dakota’s operation is to bypass parsing phases and directly populate the ProblemDescDB with information on the methods, variables, interface, responses, etc., that define the Dakota analysis problem. This approach requires more interaction with Dakota classes and data structures. However, it can offer usability benefit when the integrating application does not want their users to interact with the full Dakota syntax, or efficiency benefit when for example there are a large number of variables to configure.

In the direct database population approach, Dakota DataMethod, DataModel, DataVariables, DataInterface, and DataResponses objects are instantiated and populated with the desired problem data. These objects are then
published to the problem database using insert_nodes(). An example of this approach is available in run_dakota_data() in library_mode.cpp, where the OPT++ Quasi-Newton method is configured to work on a plugin version of text_book or rosenbrock. The data objects are populated with their default values upon instantiation and are often sufficient for basic Dakota studies. Only the non-default values need to be specified. Moreover the default Dakota Model is a SingleModel, so this object need not be configured unless tailoring its configuration or using a more advanced model type. Refer to the DataMethod, DataModel, DataVariables, DataInterface, and DataResponses class documentation and source code for lists of attributes and their defaults. Here is an excerpt of run_dakota_data() that specifies the OPT++ solver after default construction of DataMethod:

```cpp
Dakota::DataMethod dme;
Dakota::DataMethodRep* dmr = dme.data_rep();
dmr->methodName = Dakota::OPTPP_QNEWTON;
```

When using direct database population, it is critical to leave the database in an open, accessible state after initial construction. In this run_dakota_data() example, a flag check_bcast_construct is passed into the LibraryEnvironment constructor, indicating that it should not finalize the database and construct Dakota objects. Moreover, it is only necessary to populate the database on rank 0 of the MPI Comm on which Dakota is running. After database objects are inserted or adjusted, the LibraryEnvironment::done_modifying_db() function must be called before proceeding to execute. This synchronizes problem data across all ranks and constructs Dakota objects needed to run the specified analysis.

```cpp
bool check_bcast_construct = false;
Dakota::LibraryEnvironment env(MPI_COMM_WORLD, opts, check_bcast_construct);
if (rank == 0)
  // insert/modify DB, then lock and proceed:
  env.done_modifying_db();
  env.execute();
```

5.3.3 Mixed mode, callbacks, and late updates

The LibraryEnvironment API also supports mixed approaches that combine the parsing of a Dakota input file (or input string literal) with direct database updates. This approach is motivated by large-scale applications where large vectors are cumbersome to specify in a Dakota input file or where later updates to an input template are needed. The example run_dakota_mixed() in library_mode.cpp demonstrates the combination of these more advanced approaches: (1) input text parsing, (2) database updates via a callback, (3) database updates via direct manipulation, and (4) further runtime updates to the Model before running.

First, a ProgramOptions class is instantiated and configured to parse either an input file or input string literal (as in earlier examples). The passed input data must contain all required inputs so the parser can validate them. Since vector data like variable values/bounds/tags, linear/nonlinear constraint coefficients/bounds, etc., are optional, these potentially large vector specifications can be omitted from the input file and updated later through the database API. Only the variable/response counts necessary for sizing, e.g.:

```cpp
method
  linear_inequality_constraints = 500

variables
  continuous_design = 1000

responses
  objective_functions = 1
  nonlinear_inequality_constraints = 100000
```

and not the lists of values are required in this case. To update or add data after this initial parse, we use the ProblemDescDB::set() family of overloaded functions, e.g.

```cpp
Dakota::RealVector drv(1000, 1.); // vector of length 1000, values initialized to 1.
problem_db.set("variables.continuous_design.initial_point", drv);
```
where the string identifiers are the same identifiers used when pulling information from the database using one of the `get_<datatype>()` functions (refer to `ProblemDescDB` for a full list). However, the supported `ProblemDescDB::set()` options are a restricted subset of the database attributes, focused on vector inputs that can be large scale.

Second, the example demonstrates a user-provided callback function which Dakota will invoke after input parsing to update `ProblemDescDB`. In `library_mode.cpp`, `callback_function()` is a user-provided post-parse callback that implements the type Dakota::DbCallbackFunction.

```
static void callback_function(Dakota::ProblemDescDB* db, void *ptr);
```

When Dakota calls this function it will pass back pointers to the `ProblemDescDB` instance and to user-provided data, so the application may convey its settings by calling methods on the `ProblemDescDB`, optionally using the provided data. An example of a user data structure is demonstrated in `callback_data`. In this case, when the `LibraryEnvironment` is constructed, it is constructed with the input data to initially parse, the callback function, and to leave it unlocked for further updates:

```
bool done_with_db = false;
Dakota::LibraryEnvironment env(opts, done_with_db,
    callback_function, &data);
```

Third, the example demonstrates changes to the database after parsing and callback-based updates. Again, these only need happen on Dakota’s rank 0 before finalizing the DB with `LibraryEnvironment::done_modifying_db()`. The example demonstrates:

1. Getting access to the database through `env.problem_description_db()`
2. Setting the database nodes to the appropriate method through `problem_db.resolve_top_method()`
3. Getting data from the DB with a get string array function: `problem_db.get_sa("interface.application.-analysis_drivers")`
4. Setting update data with `problem_db.set("variables.continuous_design.initial_point", ip);`

After any of these three types updates, calling `LibraryEnvironment::done_modifying_db()` will broadcast any updates (including potentially large vector data and post-process specification data to fill in any vector defaults that have not yet been provided through either file parsing or direct updates. (Note: scalar defaults are handled in the Data class constructors.)

Fourth and finally, `run_dakota_mixe()` demonstrates modifying a Model’s data after database operations and interface plugin are complete. This involves finding the right Model (or other class) instance to modify, and directly adjusting its data through the public API. Since the database is finalized, any updates must be performed through direct set operations on the constructed objects. For example, to update other data such as variable values/bounds/tags or response bounds/targets/tags, refer to the set functions documented in Iterator and Model.

As an example, the following code updates the active continuous variable values, which will be employed as the initial guess for certain classes of Iterators:

```
ModelList& all_models = problem_db.model_list();
Model& first_model = *all_models.begin();
Dakota::RealVector drv(1000, 1.); // vector of length 1000, values initialized to 1.
first_model.continuous_variables(drv);
```
CHAPTER 5. INTERFACING WITH DAKOTA AS A LIBRARY

Remarks

If performing such data updates within the constructor of a DirectApplicInterface extension/derivation (see Creating a simulator plugin interface), then this code is sufficient since the database is unlocked, the active list nodes of the ProblemDescDB have been set for you, and the correct method/model/variables/interface/responses specification instance will get updated. The difficulty in this case stems from the order of instantiation. Since the Variables and Response instances are constructed in the base Model class, prior to construction of Interface instances in derived Model classes, database information related to Variables and Response objects will have already been extracted by the time the Interface constructor is invoked and the database update will not propagate.

Therefore, it is preferred to perform these database set operations at a higher level (e.g., within your main program), prior to allowing Environment to broadcast, construct, and execute, such that instantiation order is not an issue. However, in this case, it is necessary to explicitly manage the list nodes of the ProblemDescDB using a specification instance identifier that corresponds to an identifier from the input file, e.g.:

```cpp
problem_db.set_db_variables_node("MY_VARIABLES_ID");
Dakota::RealVector drv(1000, 1); // vector of length 1000, values initialized to 1.
problem_db.set("variables.continuous_design.initial_point", drv);
```

Alternatively, rather than setting just a single data node, all data nodes may be set using a method specification identifier:

```cpp
problem_db.set_db_list_nodes("MY_METHOD_ID");
```

since the method specification is responsible for identifying a model specification, which in turn identifies variables, interface, and responses specifications. If hard-wiring specification identifiers is undesirable, then

```cpp
problem_db.resolve_top_method();
```

can also be used to deduce the active method specification and set all list nodes based on it. This is most appropriate in the case where only single specifications exist for method/model/variables/interface/responses. This is the approach demonstrated in run_dakotamixed(). In each of these cases, setting list nodes unlocks the corresponding portions of the database, allowing set/get operations.

5.4 Creating a simulator plugin interface

The DirectApplicInterface class provides an interface for Dakota to call the simulation code directly to perform function evaluations mapping variables to responses. This provides the "back end" for Dakota to call back to the simulation framework. Two approaches to defining this direct interface are described here. The first is less common, while the second is recommended when possible.

5.4.1 Extension

The first approach involves extending one of the existing DirectApplicInterface subclasses (TestDriverInterface, MatlabInterface, etc.) to support additional direct simulation interfaces. For example, Dakota algebraic test problems are implemented in TestDriverInterface. One could add additional direct functions to Dakota in TestDriverInterface::derived_map_ac(). In addition, TestDriverInterface::derived_map_if() and TestDriverInterface::derived_map_of() can be extended to perform pre- and post-processing tasks if desired, but this is not required.

While this approach is the simplest, it has the disadvantage that the Dakota library will need to be recompiled when the simulation or its direct interface is modified. If it is desirable to maintain the independence of the Dakota library from the host application, then the derivation approach described in the next section should be employed.
5.4. CREATING A SIMULATOR PLUGIN INTERFACE

Remarks

If the new direct evaluation function implementation will not be a member function of one of the Dakota classes, then the following prototype should be used in order to pass the required data:

```cpp
int sim(const Dakota::Variables& vars, const Dakota::ActiveSet& set, Dakota::Response& response);
```

If the new function will be a member function, e.g., in TestDriverInterface, then this can be simplified to

```cpp
int sim();
```

since the data access can be performed through the DirectApplicInterface class attributes.

5.4.2 Derivation

The second approach is to derive a new interface from DirectApplicInterface and redefine several virtual functions. As demonstrated in SIM::SerialDirectApplicInterface and SIM::ParallelDirectApplicInterface, a typical derived class declaration might be

```cpp
namespace SIM {
  class SerialDirectApplicInterface: public Dakota::DirectApplicInterface {
    public:
      // Constructor and destructor
      SerialDirectApplicInterface(const Dakota::ProblemDescDB& problem_db);
      ~SerialDirectApplicInterface();

    protected:
      // Virtual function redefinitions
      int derived_map_if(const Dakota::String& if_name);
      int derived_map_ac(const Dakota::String& ac_name);
      int derived_map_of(const Dakota::String& of_name);

    private:
      // Data
    }
  } // namespace SIM
```

where the new derived class resides in the simulation’s namespace. Similar to the case of Extension, the DirectApplicInterface::derived_map_ac() function is the required redefinition, and DirectApplicInterface::derived_map_if() and DirectApplicInterface::derived_map_of() are optional.

Typically the new derived_map_ac() implementation delegates to the main simulation application for a function evaluation. Here Dakota variables would get mapped into the simulation’s data structures, the simulation executed, and derived response data computed for return to Dakota.

Once a derived application class is created, it must be plugged in, or registered, with the appropriate Interface in the LibraryEnvironment. In MPI cases where Dakota is potentially managing concurrent evaluations of the simulation, the plugin must be configured to run on the right MPI sub-communicator, or Dakota analysis comm. The simpler case is demonstrated in serial_interface_plugin() in library_mode.cpp, while a more advanced case using the analysis communicator is shown in parallel_interface_plugin().

The Dakota LibraryEnvironment provides a convenience function to plugin an Interface. This example will replace any interface found matching the given model, interface, and analysis driver with the passed plugin interface:
std::string model_type("" data: empty string will match any model type
std::string interf_type("direct");
std::string an_driver("plugin_rosenbrook");
Dakota::ProblemDescDB* problem_db = env.problem_description_db();
Dakota::Interface* serial_iface =
    new SIM::SerialDirectApplicInterface(problem_db);
bool plugged_in =
    env.plugin_interface(model_type, interf_type, an_driver, serial_iface);

The LibraryEnvironment also provides convenience functions that allow the client to iterate the lists of available interfaces or models for more advanced cases. For instance if the client knows there is only a single interface active, it could get the list of available interfaces of length 1 and plug into the first one. In the more advanced case where the simulation interface instance should manage parallel simulations within the context of an MPI communicator, one should pass in the relevant analysis communicator(s) to the derived constructor. For the latter case of looping over a set of models, the simplest approach of passing a single analysis communicator would use code similar to

Dakota::ModelList filt_models =
    env.filtered_model_list("single", "direct", "plugin_text_book");
Dakota::ProblemDescDB* problem_db = env.problem_description_db();
Dakota::ModelList ml_iter;
for (ml_iter = filt_models.begin(); ml_iter != filt_models.end(); ++ml_iter) {
    // set DB nodes to input specification for this Model
    problem_db.set_db_model_nodes(ml_iter->model_id());

    // Parallel case: plug in derived Interface object with an analysisComm.
    // Note: retrieval and passing of analysisComm is necessary only if
    // parallel operations will be performed in the derived constructor.
    const MPI_Comm& analysis_comm = ml_iter->analysis_comm();
    // don’t increment ref count since no other envelope shares this letter
    ml_iter.derived_interface.assign_rep(new SIM::ParallelDirectApplicInterface(problem_db, analysis_comm), false);}

The file library_mode.cpp demonstrates each of these approaches. Since a Model may be used in multiple parallel contexts and may therefore have a set of parallel configurations, a more general approach would extract and pass an array of analysis communicators to allow initialization for each of the parallel configurations.

New derived direct interface instances inherit various attributes of use in configuring the simulation. In particular, the ApplicationInterface::parallelLib reference provides access to MPI communicator data (e.g., the analysis communicators discussed above), DirectApplicInterface::analysisDrivers provides the analysis driver names specified by the user in the input file, and DirectApplicInterface::analysisComponents provides additional analysis component identifiers (such as mesh file names) provided by the user which can be used to distinguish different instances of the same simulation interface. It is worth noting that inherited attributes that are set as part of the parallel configuration (instead of being extracted from the ProblemDescDB) will be set to their defaults following construction of the base class instance for the derived class plug-in. It is not until run-time (i.e., within derived_map/derived_map_ac/derived_map_of) that the parallel configuration settings are re-propagated to the plug-in instance. This is the reason that the analysis communicator should be passed in to the constructor of a parallel plug-in, if the constructor will be responsible for parallel application initialization.
5.5 Retrieving data after a run

After executing the Dakota Environment, final results can be obtained through the use of Environment::variables_results() and Environment::response_results(), e.g.:

```cpp
// retrieve the final parameter values
const Variables& vars = env.variables_results();

// retrieve the final response values
const Response& resp = env.response_results();
```

In the case of optimization, the final design is returned, and in the case of uncertainty quantification, the final statistics are returned. Dakota has a prototype results database, which will eventually provide better access to the results from a study.

5.6 Linking against the Dakota library

This section presumes Dakota has been configured with CMake, compiled, and installed to a CMAKE_INSTALL_PREFIX using make install or equivalent. The Dakota libraries against which you must link will typically install to CMAKE_INSTALL_PREFIX/bin/ and CMAKE_INSTALL_PREFIX/lib/, while headers are provided in CMAKE_INSTALL_PREFIX/lib/. The core Dakota C and C++ code is in the library dakota_src, while Fortran code lives in the dakota_src_fortran library. Runtime libraries for any configure-enabled Dakota third-party software components (such as DOT, NPSOL, OPT++, LHS, etc.) are also installed to the lib/ directory. Applications link against these Dakota libraries by specifying appropriate include and link directives.

There two primary ways to determine the necessary Dakota-related libraries and link order for linking your application. First, when running CMake, a list of required Dakota and Dakota-included third-party libraries will be output to the console, e.g.,

```
-- Dakota_LIBRARIES: dakota_src;dakota_src_fortran;nidr;teuchos;pecos;pecos_src;lhs;mods;mod;fftpack;sparsel
```

While external dependencies will be output as:

```
-- Dakota_TPL_LIBRARIES: /usr/lib64/libcurl.so;/usr/lib64/openmpi/lib/libmpi_cxx.so;debug;/usr/lib64/libz.so;
```

Note that depending on how you configured Dakota, some libraries may be omitted from these lists (for example commercial add-ons NPSOL, DOT, and NLPQL), or additional libraries may appear.

A second option is to check which libraries appear in CMAKE_INSTALL_PREFIX/bin/ CMAKE_INSTALL_PREFIX/lib/, or more accurately, see the file Makefile.export.Dakota in the Dakota build/src/ or installation include/ directory. Here are some additional notes on specific libraries:

- Some Boost libraries (boost_regex, boost_filesystem, boost_system, boost_serialization) are required, and other Boost library components may be required depending on configuration, e.g., boost_system_signals when configuring with HAVE_ACRO_BOOL=TRUE
- System compiler and math libraries may need to be included, as may additional system libraries such as Expat and Curl, depending on how Dakota is configured.
- If configuring with graphics, you will need to add the dakota_sciplot library and system X libraries (partial list here):

```
-lXpm -lXm -lXt -lXmu -lXp -lXext -lX11 -lSM -lICE
```
• When configuring with AMPL (HAVEAMPL:BOOL=ON), the AMPL solver library may require dl, funcadd0.o and fl libraries. We have experienced problems with the creation of libamplsolver.a on some platforms; use the dakota-users mailing list to get help with any problems related to this.

• Optional library GSL (discouraged due to GPL license) and if linking with system-provided GSL, gslcblas may be needed if Dakota was configured with them.

• Newmat: as of Dakota 5.2, -lnewmat is no longer required

Finally, it is important to use the same C++ compiler (possibly an MPI wrapper) for compiling Dakota and your application and potentially include Dakota-related preprocessor defines as emitted by CMake during compilation of Dakota and included in Makefile.export.Dakota. This ensures that the platform configuration settings are properly synchronized across Dakota and your application.
Performing function evaluations is one of the most critical functions of the Dakota software. It can also be one of the most complicated, as a variety of scheduling approaches and parallelism levels are supported. This complexity manifests itself in the code through a series of cascaded member functions, from the top level model evaluation functions, through various scheduling routines, to the low level details of performing a system call, fork, or direct function invocation. This section provides an overview of the primary classes and member functions involved.

### 6.1 Synchronous function evaluations

For a synchronous (i.e., blocking) mapping of parameters to responses, an iterator invokes `Model::evaluate()` to perform a function evaluation. This function is all that is seen from the iterator level, as underlying complexities are isolated. The binding of this top level function with lower level functions is as follows:

- `Model::evaluate()` utilizes `Model::derived_evaluate()` for portions of the response computation specific to derived model classes.
- `Model::derived_evaluate()` directly or indirectly invokes `Interface::map()`.
- `Interface::map()` utilizes `ApplicationInterface::derived_map()` for portions of the mapping specific to derived application interface classes.

### 6.2 Asynchronous function evaluations

For an asynchronous (i.e., nonblocking) mapping of parameters to responses, an iterator invokes `Model::evaluate_nowait()` multiple times to queue asynchronous jobs and then invokes either `Model::synchronize()` or `Model::synchronize_nowait()` to schedule the queued jobs in blocking or nonblocking fashion. Again, these functions are all that is seen from the iterator level, as underlying complexities are isolated. The binding of these top level functions with lower level functions is as follows:

- `Model::evaluate_nowait()` utilizes `Model::derived_evaluate_nowait()` for portions of the response computation specific to derived model classes.
- This derived model class function directly or indirectly invokes `Interface::map()` in asynchronous mode, which adds the job to a scheduling queue.
- `Model::synchronize()` or `Model::synchronize_nowait()` utilize `Model::derived_synchronize()` or `Model::derived_synchronize_nowait()` for portions of the scheduling process specific to derived model classes.
• These derived model class functions directly or indirectly invoke Interface::synch() or Interface::synch_no- 
nowait().

• For application interfaces, these interface synchronization functions are responsible for performing evalu-
ation scheduling in one of the following modes: master dynamic, peer dynamic or peer static.

• NOTE: The Interface evaluation scheduling in Dakota was refactored for releases 5.4 and 6.0. Discussion of the 
new Interface-related functions is currently missing here.

6.3 Analyses within each function evaluation

NOTE: The Interface evaluation scheduling in Dakota was refactored for releases 5.4 and 6.0. Discussion of the 
new Interface-related functions for analyses is currently missing here.

The discussion above covers the parallelism level of concurrent function evaluations serving an iterator. For 
the parallelism level of concurrent analyses serving a function evaluation, similar schedulers are involved 
to support synchronous local, asynchronous local, message passing, and hybrid modes. Not all of the sched-
ulers are elevated to the ApplicationInterface level since the system call and direct function interfaces do not yet support nonblocking local analyses (and therefore support synchronous local and message passing modes, but not asynchronous local or hybrid modes). Fork interfaces, however, support all modes of analysis parallelism.
Chapter 7

Working with Variable Containers and Views

Variable views control the subset of variable types that are active and inactive within a particular iterative study. For design optimization and uncertainty quantification (UQ), for example, the active variables view consists of design or uncertain types, respectively, and any other variable types are carried along invisible to the iterative algorithm being employed. For parameter studies and design of experiments, however, a variable subset view is not imposed and all variables are active. Selected UQ methods can also be toggled into an “All” view using the active all variables input specification. When not in an All view, finer gradations within the uncertain variable sets are also relevant: probabilistic methods (reliability, stochastic expansion) view aleatory uncertain variables as active, nonprobabilistic methods (interval, evidence) view epistemic uncertain variables as active, and a few UQ methods (sampling) view both as active. In a more advanced NestedModel use case such as optimization under uncertainty, design variables are active in the outer optimization context and the uncertain variables are active in the inner UQ context, with an additional requirement on the inner UQ level to return derivatives with respect to its “inactive” variables (i.e., the design variables) for use in the outer optimization loop.

For efficiency, contiguous arrays of data store variable information for each of the domain types (continuous, discrete integer, and discrete real), but active and inactive views into them permit selecting subsets in a given context. This management is encapsulated into the Variables and SharedVariablesData classes. This page clarifies concepts of relaxed (formerly merged) vs. mixed, fine-grained vs. aggregated types, domain types, and views into contiguous arrays.

We begin with an overview of the storage and management concept, for which the following two sections describe the storage of variable values and meta-data about their organization, used in part to manage views. They are intended to communicate rationale to maintainers of Variables and SharedVariablesData classes. The final section provides a discussion of active and inactive views.

7.1 Storage in Variables

As described in the Main Page Variables, a Variables object manages variable types (design, aleatory uncertain, epistemic uncertain, and state) and domain types (continuous, discrete integer, and discrete real) and supports different approaches to either distinguishing among these types or aggregating them. Two techniques are used in cooperation to accomplish this management: (1) class specialization (RelaxedVariables or MixedVariables) and (2) views into contiguous variable arrays. The latter technique is used whenever it can satisfy the requirement, with fallback to class specialization when it cannot. In particular, aggregation or separation of variable types can be accomplished with views, but for aggregation or separation of variable domains, we must resort to class
specialization in order to relax discrete domain types. In this class specialization, a `RelaxedVariables` object combines continuous and discrete types (relaxing integers to reals) whereas a `MixedVariables` object maintains the integer/real distinction throughout.

The core data for a `Variables` instance is stored in a set of three contiguous arrays, corresponding to the domain types: `allContinuousVars`, `allDiscreteIntVars`, and `allDiscreteRealVars`, unique to each `Variables` instance.

Within the core variable data arrays, data corresponding to different aggregated variable types are stored in sequence for each domain type:

- continuous: [design, aleatory uncertain, epistemic uncertain, state]
- discrete integer: [design, aleatory uncertain, (epistemic uncertain), state]
- discrete real: [design, aleatory uncertain, (epistemic uncertain), state]

Note there are currently no epistemic discrete variables. This domain type ordering (continuous, discrete integer, discrete real) and aggregated variable type ordering (design, aleatory uncertain, epistemic uncertain, state) is preserved whenever distinct types are flattened into single contiguous arrays. Note that the aleatory and epistemic uncertain variables contain sub-types for different distributions (e.g., normal, uniform, histogram, poisson), and discrete integer types include both integer ranges and integer set sub-types. All sub-types are ordered according to their order of appearance in `dakota.input.nspec`.

When relaxing in `MixedVariables`, the `allContinuousVars` will also aggregate the discrete types, such that they contain ALL design, then ALL uncertain, then ALL state variables, each in aggregated type order; the `allDiscreteIntVars` and `allDiscreteRealVars` arrays are empty.

### 7.2 Storage in SharedVariablesData

Each `Variables` instance contains a reference-counted `SharedVariablesData` object that stores information on the variables configuration. This configuration data includes counts, types, IDs, and labels, which are often the same across many `Variables` instances. Thus, `SharedVariablesData` is intended to reduce the memory footprint by allowing the sharing of a single copy of redundant information among different `Variables` instances.

One of the purposes of this shared information is to support mappings between variable types, IDs, and indices into the storage arrays. Variable "types" refer to the fine-grained variable types a user would specify in an input file, as enumerated in `DataVariables.hpp`, e.g., `CONTINUOUS`, `DESIGN`, `WEIBULL`, `UNCERTAIN`, `DISCRETE`, `STATE`, `RANGE`, etc. `variablesComponents` is a map from these variable types to counts of how many are present.

In contrast, the `variablesCompsTotals` array stores total counts of each "aggregated type" (design, aleatory uncertain, epistemic uncertain, state) which might be selected to be active in a given view. Thus this array has length 12 to track the combinations of three domain type storage arrays with four possible aggregated variable types: `{continuous, discrete integer, discrete real} x {design, aleatory uncertain, epistemic uncertain, state}`. For example, the first entry of this array stores the number of continuous design variables, the second the number of discrete integer design (including both discrete design range and discrete design set integer types), and the last the number of discrete real state variables.

The arrays `allContinuousTypes`, `allDiscreteIntTypes`, and `allDiscreteRealTypes` are sized to match the corresponding core domain type storage arrays. They track the fine-grained variable type stored in that entry of the data array (since when relaxed, the continuous array may be storing data corresponding to discrete data).

Finally `allContinuousIds` stores the 1-based IDs of the variables stored in the `allContinuousVars` array, i.e., the variable number of all the problem variables considered as a single contiguous set, in aggregate type order. For relaxed (formerly merged) views, `relaxedDiscreteIds` stores the 1-based IDs of the variables which have been relaxed into the continuous array.
7.3. ACTIVE AND INACTIVE VIEWS

These counts, types, and IDs are most commonly used within the Model classes for mappings between variables objects at different levels of a model recursion. See, for example, the variable mappings in the NestedModel constructor.

7.3 Active and inactive views

The pair SharedVariablesDataRep::variablesView tracks the active and inactive views of the data, with values taken from the enum in DataVariables.hpp. The valid values include EMPTY and the combinations {relaxed, mixed} \times \{all, design, aleatory uncertain, epistemic uncertain, uncertain, state\}. The ALL cases indicate aggregation of the design, aleatory uncertain, epistemic uncertain, and state types, whereas the DISTINCT cases indicate either no aggregation (design, aleatory uncertain, epistemic uncertain, state) or reduced aggregation (aleatory+epistemic uncertain). The active view is determined by the algorithm in use, managed in Variables::get_view(). Any inactive view is set based on higher level iteration within a model recursion (e.g., a NestedModel), which enables lower level iteration to return derivatives with respect to variables that are active at the higher level. In the case where there is no higher level iteration, then the inactive view will remain EMPTY. It is important to stress that "inactive" at one level corresponds to active at another, and therefore the inactive set of variables should not be interpreted as the strict complement of the active set of variables; rather, active and inactive are both subsets whose union may still be a subset of the total container (more precise terminology might involve "primary" active and "secondary" active or similar). An active complement view could potentially be supported in the future, should the need arise, although this view would require management of non-contiguous portions of the aggregated arrays.

Given these groupings (views), the active and inactive subsets of the allContinuousVars, allDiscreteIntVars, and allDiscreteRealVars arrays are always contiguous, permitting vector views of the underlying data using either Teuchos::View (for numerical vectors) or Boost.MultiArray (for book-keeping arrays) views.

When a Variables envelope is constructed, its letter is initialized to either a RelaxedVariables or MixedVariables object depending on the active view. The derived classes size the contiguous storage arrays to accommodate all the problem variables, and then initialize active views into them, which could involve either subsets (DISTINCT active views) or views of the full arrays (ALL active views). Inactive views, on the other hand, are initialized during construction of a model recursion (e.g., a call to Model::inactive_view() in the NestedModel constructor). Thus, active variable subsets are always available but inactive variable subsets will be EMPTY prior to them being initialized within a Model recursion.

Accessors for continuous variables include:

- continuous_variables(): returns the active view which might return all (ALL views) or a subset (DISTINCT views) such as design, uncertain, only aleatory uncertain, etc.
- inactive_continuous_variables(): returns the inactive view which is either a subset or empty
- all_continuous_variables(): returns the full vector allContinuousVars

and this pattern is followed for active/inactive/all access to discrete_int_variables() and discrete_real_variables() as well as for labels, IDs, and types in SharedVariablesData and variable bounds in Constraints.

Member SurfpackApproximation::build ()

Right now, we’re completely deleting the old data and then recopying the current data into a SurfData object. This was just the easiest way to arrive at a solution that would build and run. This function is frequently called from addPoint rebuild, however, and it’s not good to go through this whole process every time one more data point is added.

Member SurfpackApproximation::hessian (const RealVector &c_vars)

Make this acceptably efficient
Member `SurfpackApproximation::hessian` (const Variables &vars)
  Make this acceptably efficient
Chapter 8

Namespace Index

8.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

- **Dakota**
  - The primary namespace for DAKOTA

- **SIM**
  - A sample namespace for derived classes that use assign_rep() to plug facilities into DAKOTA
9.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

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VLstr
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Chapter 11

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11.1 File List

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- **dakota_dll_api.cpp**
  - This file contains a DakotaRunner class, which launches DAKOTA
  - Line: 921

- **dakota_dll_api.h**
  - API for DLL interactions
  - Line: 922

- **dakota_linear_algebra.hpp**
  - Dakota linear algebra utilities
  - Line: 923

- **dakota_tabular_io.hpp**
  - Utility functions for reading and writing tabular data files
    Emerging utilities for tabular file I/O. For now, just extraction of capability from separate contexts to facilitate rework. These augment (and leverage) those in data_util.h
  - Line: 924

- **dll_tester.cpp**
  - Test the DLL with a DAKOTA input file
  - Line: 926

- **JEGAOptimizer.cpp**
  - Contains the implementation of the JEGAOptimizer class
  - Line: 926

- **JEGAOptimizer.hpp**
  - Contains the definition of the JEGAOptimizer class
  - Line: 927

- **library_mode.cpp**
  - File containing a mock simulator main for testing Dakota in library mode
  - Line: 928

- **library_split.cpp**
  - File containing a mock simulator main for testing DAKOTA in library mode on a split communicator
  - Line: 931

- **main.cpp**
  - File containing the main program for DAKOTA
  - Line: 932

- **restart_util.cpp**
  - File containing the DAKOTA restart utility main program
  - Line: 932
Chapter 12

Namespace Documentation

12.1 Dakota Namespace Reference

The primary namespace for DAKOTA.

Classes

- class ActiveSubspaceModel
  
  Active subspace model for input (variable space) reduction.

- class AdaptedBasisModel
  
  Adapted basis model for input (variable space) reduction.

- class ApplicationInterface
  
  Derived class within the interface class hierarchy for supporting interfaces to simulation codes.

- class ApproximationInterface
  
  Derived class within the interface class hierarchy for supporting approximations to simulation-based results.

- class APPSEvalMgr
  
  Evaluation manager class for APPSPACK.

- class APPSOptimizer
  
  Wrapper class for HOPSPACK.

- class BootstrapSamplerBase
  
  Base class/interface for the bootstrap sampler.

- class BootstrapSampler
  
  Actual bootstrap sampler implementation for common data types.

- class BootstrapSampler<Teuchos::SerialDenseMatrix<OrdinalType, ScalarType>>
  
  Bootstrap sampler that is specialized to allow for the bootstrapping of RealMatrix.

- class BootstrapSamplerWithGS
  
  A derived sampler to allow for user specification of the accessor methods.

- class COLINApplication

- class COLINOptimizer
  
  Wrapper class for optimizers defined using COLIN.

- class CollabHybridMetaIterator
  
  Meta-iterator for hybrid iteration using multiple collaborating optimization and nonlinear least squares methods.
• class GetLongOpt
  
  GetLongOpt is a general command line utility from S. Manoharan (Advanced Computer Research Institute, Lyon, France).

• class CommandLineHandler
  Utility class for managing command line inputs to DAKOTA.

• class CommandShell
  Utility class which defines convenience operators for spawning processes with system calls.

• class ConcurrentMetaIterator
  Meta-iterator for multi-start iteration or pareto set optimization.

• class CONMINOptimizer
  Wrapper class for the CONMIN optimization library.

• class FileReadException
  base class for Dakota file read exceptions (to allow catching both tabular and general file truncation issues)

• class TabularDataTruncated
  exception thrown when data read truncated

• class ResultsFileError
  exception throw for other results file read error

• class FunctionEvalFailure
  exception class for function evaluation failures

• struct BaseConstructor
  Dummy struct for overloading letter-envelope constructors.

• struct NoDBBaseConstructor
  Dummy struct for overloading constructors used in on-the-fly instantiations without ProblemDescDB support.

• struct LightWtBaseConstructor
  Dummy struct for overloading constructors used in on-the-fly Model instantiations.

• class ActiveSet
  Container class for active set tracking information. Contains the active set request vector and the derivative variables vector.

• class Analyzer
  Base class for NonD, DACE, and ParamStudy branches of the iterator hierarchy.

• class Approximation
  Base class for the approximation class hierarchy.

• class Constraints
  Base class for the variable constraints class hierarchy.

• class Environment
  Base class for the environment class hierarchy.

• class Graphics
  The Graphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics; there is only one instance of this
  OutputManager::dakotaGraphics.

• class Interface
  Base class for the interface class hierarchy.

• class Iterator
  Base class for the iterator class hierarchy.

• class LeastSq
12.1. DAKOTA NAMESPACE REFERENCE

Base class for the nonlinear least squares branch of the iterator hierarchy.
- class Minimizer
  Base class for the optimizer and least squares branches of the iterator hierarchy.
- class ScalingOptions
  Simple container for user-provided scaling data, possibly expanded by replicates through the models.
- class Model
  Base class for the model class hierarchy.
- class NonD
  Base class for all nondeterministic iterators (the DAKOTA/UQ branch).
- class Optimizer
  Base class for the optimizer branch of the iterator hierarchy.
- class PStudyDACE
  Base class for managing common aspects of parameter studies and design of experiments methods.
- class Response
  Container class for response functions and their derivatives. Response provides the enveloper base class.
- class GeneralReader
  Utility used in derived read_core to read in generic format.
- class TabularReader
  Utility used in derived read_core to read values in tabular format.
- class GeneralWriter
  Utility used in derived write_core to write in generic format.
- class ApreproWriter
  Utility used in derived write_core to write in aprepro format.
- class TabularWriter
  Utility used in derived write_core to write values in tabular format.
- class LabelsWriter
  Utility used in derived write_core to write labels in tabular format.
- class Variables
  Base class for the variables class hierarchy.
- class Verification
  Base class for managing common aspects of verification studies.
- class DataEnvironmentRep
  Body class for environment specification data.
- class DataEnvironment
  Handle class for environment specification data.
- class DataFitSurrBasedLocalMinimizer
  Class for provably-convergent local surrogate-based optimization and nonlinear least squares.
- class DataFitSurrModel
  Derived model class within the surrogate model branch for managing data fit surrogates (global and local)
- class DataInterface
  Handle class for interface specification data.
- class DataMethodRep
  Body class for method specification data.
• class DataMethod
  Handle class for method specification data.
• class DataModelRep
  Body class for model specification data.
• class DataModel
  Handle class for model specification data.
• class DataResponsesRep
  Body class for responses specification data.
• class DataResponses
  Handle class for responses specification data.
• class DataTransformModel
  Data transformation specialization of RecastModel.
• class DataVariablesRep
  Body class for variables specification data.
• class DataVariables
  Handle class for variables specification data.
• class DDACEDesignCompExp
  Wrapper class for the DDACE design of experiments library.
• class DirectApplicInterface
  Derived application interface class which spawns simulation codes and testers using direct procedure calls.
• class DiscrepancyCorrection
  Base class for discrepancy corrections.
• class DOTOptimizer
  Wrapper class for the DOT optimization library.
• class EffGlobalMinimizer
  Implementation of Efficient Global Optimization/Least Squares algorithms.
• class EmbedHybridMetaIterator
  Meta-iterator for closely-coupled hybrid iteration, typically involving the embedding of local search methods within global search methods.
• class ExecutableEnvironment
  Environment corresponding to execution as a stand-alone application.
• class ExperimentData
  Interpolation method for interpolating between experimental and model data. I need to work on inputs/outputs to this method. For now, this assumes interpolation of functional data.
• class ExperimentResponse
  Container class for response functions and their derivatives. ExperimentResponse provides the body class.
• class ForkApplicInterface
  Derived application interface class which spawns simulation codes using fork/execvp/waitpid.
• class FSUDesignCompExp
  Wrapper class for the FSUDace QMC/CVT library.
• class GaussProcApproximation
  Derived approximation class for Gaussian Process implementation.
• class GridApplicInterface
12.1. DAKOTA NAMESPACE REFERENCE

Derived application interface class which spawns simulation codes using grid services such as Condor or Globus.

- class HierarchSurrBasedLocalMinimizer
  Class for multilevel-multifidelity optimization algorithm.

- class HierarchSurrModel
  Derived model class within the surrogate model branch for managing hierarchical surrogates (models of varying fidelity).

- class IteratorScheduler
  This class encapsulates scheduling operations for concurrent sub-iteration within an outer level context (e.g., meta-iteration, nested models).

- class JEGAOptimizer
  A version of Dakota::Optimizer for instantiation of John Eddy’s Genetic Algorithms (JEGA).

- class LibraryEnvironment
  Environment corresponding to execution as an embedded library.

- class MatlabInterface

- class MetaIterator
  Base class for meta-iterators.

- class MixedVarConstraints
  Derived class within the Constraints hierarchy which separates continuous and discrete variables (no domain type array merging).

- class MixedVariables
  Derived class within the Variables hierarchy which separates continuous and discrete variables (no domain type array merging).

- class MPIManager
  Class MPIManager to manage Dakota’s MPI world, which may be a subset of MPI_COMM_WORLD.

- class MPIPackBuffer
  Class for packing MPI message buffers.

- class MPIUnpackBuffer
  Class for unpacking MPI message buffers.

- class NCSUOptimizer
  Wrapper class for the NCSU DIRECT optimization library.

- class NestedModel
  Derived model class which performs a complete sub-iterator execution within every evaluation of the model.

- struct Var_rcheck
  structure for verifying bounds and initial point for real-valued vars

- struct Var_icheck
  structure for verifying bounds and initial point for string-valued vars

- struct VLreal
  structure for validating real uncertain variable labels, bounds, values

- struct VLint
  structure for validating integer uncertain variable labels, bounds, values

- struct VLstr
  structure for validating string uncertain variable labels, bounds, values

- class NIDRProblemDescDB
  The derived input file database utilizing the new IDR parser.
• struct NL2Res
  Auxiliary information passed to calcr and calcj via ur.
• class NL2SOLLeastSq
  Wrapper class for the NL2SOL nonlinear least squares library.
• class NLPQLPOptimizer
  Wrapper class for the NLPQLP optimization library, Version 2.0.
• class NLSSOLLeastSq
  Wrapper class for the NLSSOL nonlinear least squares library.
• class NomadOptimizer
  Wrapper class for NOMAD Optimizer.
• class NonDAdaptImpSampling
  Class for the Adaptive Importance Sampling methods within DAKOTA.
• class NonDAdaptiveSampling
  Class for testing various Adaptively sampling methods using geometric, statistical, and topological information of the surrogate.
• class NonDBayesCalibration
  Base class for Bayesian inference: generates posterior distribution on model parameters given experimental data.
• class NonDCalibration
• class NonDCubature
  Derived nondeterministic class that generates N-dimensional numerical cubature points for evaluation of expectation integrals.
• class NonDDREAMBayesCalibration
  Bayesian inference using the DREAM approach.
• class NonDExpansion
  Base class for polynomial chaos expansions (PCE) and stochastic collocation (SC)
• class NonDGlobalEvidence
  Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.
• class NonDGlobalInterval
  Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.
• class NonDGlobalReliability
  Class for global reliability methods within DAKOTA/UQ.
• class NonDGlobalSingleInterval
  Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.
• class NonDGPImpSampling
  Class for the Gaussian Process-based Importance Sampling method.
• class NonDGPSABayesCalibration
  Generates posterior distribution on model parameters given experiment data.
• class NonDIntegration
  Derived nondeterministic class that generates N-dimensional numerical integration points for evaluation of expectation integrals.
• class NonDInterval
  Base class for interval-based methods within DAKOTA/UQ.
12.1. DAKOTA NAMESPACE REFERENCE

• class NonDLHSEvidence
  
  Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

• class NonDLHSInterval
  
  Class for the LHS-based interval methods within DAKOTA/UQ.

• class NonDLHSSampling
  
  Performs LHS and Monte Carlo sampling for uncertainty quantification.

• class NonDLHSSingleInterval
  
  Class for pure interval propagation using LHS.

• class NonDLocalEvidence
  
  Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

• class NonDLocalInterval
  
  Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

• class NonDLocalReliability
  
  Class for the reliability methods within DAKOTA/UQ.

• class NonDLocalSingleInterval
  
  Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

• class NonDMultilevelSampling
  
  Performs Multilevel Monte Carlo sampling for uncertainty quantification.

• class NonDPOFDarts
  
  Base class for POF Dart methods within DAKOTA/UQ.

• class NonDPolynomialChaos
  
  Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

• class NonDQuadrature
  
  Derived nondeterministic class that generates N-dimensional numerical quadrature points for evaluation of expectation integrals over uncorrelated standard normals/uniforms/exponentials/betas/gammas.

• class QuesoJointPdf
  
  Dakota specialization of QUESO generic joint PDF.

• class QuesoVectorRV
  
  Dakota specialization of QUESO vector-valued random variable.

• class NonDQUESOBayesCalibration
  
  Bayesian inference using the QUESO library from UT Austin.

• class NonDReliability
  
  Base class for the reliability methods within DAKOTA/UQ.

• class NonDRKDDarts
  
  Base class for the Recursive k-d Dart methods within DAKOTA/UQ.

• class NonDSampling
  
  Base class for common code between NonDLHSSampling, NonDAdaptImpSampling, and other specializations.

• class NonDSparseGrid
  
  Derived nondeterministic class that generates N-dimensional Smolyak sparse grids for numerical evaluation of expectation integrals over independent standard random variables.

• class NonDStochCollocation
  
  Nonintrusive stochastic collocation approaches to uncertainty quantification.
• class NonDWASABIBayesCalibration
  WASABI - Weighted Adaptive Surrogate Approximations for Bayesian Inference.
• class NonlinearCGOptimizer
• class NOWPACBlackBoxEvaluator
  Derived class for plugging Dakota evaluations into NOWPAC solver.
• class NOWPACOptimizer
  Wrapper class for the (S)NOWPAC optimization algorithms from Florian Augustin (MIT)
• class NPSOLOptimizer
  Wrapper class for the NPSOL optimization library.
• class OptDartsOptimizer
  Wrapper class for OptDarts Optimizer.
• class OutputWriter
• class ConsoleRedirector
• class RestartWriter
• class OutputManager
  Class to manage redirection of stdout/stderr, keep track of current redir state, and manage rank 0 output. Also manage tabular data output for post-processing with Matlab, Tecplot, etc. and delegate to Graphics for X Windows Graphics.
• class ParallelLevel
  Container class for the data associated with a single level of communicator partitioning.
• class ParallelConfiguration
  Container class for a set of ParallelLevel list iterators that collectively identify a particular multilevel parallel configuration.
• class ParallelLibrary
  Class for partitioning multiple levels of parallelism and managing message passing within these levels.
• class ParamResponsePair
  Container class for a variables object, a response object, and an evaluation id.
• class ParamStudy
  Class for vector, list, centered, and multidimensional parameter studies.
• class PebbldBranching
  Main Branching class for the PEBBL-based Minimizer.
• class PebbldBranchSub
  Sub Branch class for the PEBBL-based Minimizer.
• class PebbldMinimizer
  Wrapper class for experimental PebbldMinimizer.
• class PecosApproximation
  Derived approximation class for global basis polynomials.
• class ProbabilityTransformModel
  Probability transformation specialization of RecastModel.
• class ProblemDescDB
  The database containing information parsed from the DAKOTA input file.
• class ProcessApplicInterface
  Derived application interface class that spawns a simulation code using a separate process and communicates with it through files.
• class ProcessHandleApplicInterface
  Derived application interface class that spawns a simulation code using a separate process, receives a process identifier, and communicates with the spawned process through files.

• class ProgramOptions
  ProgramOptions stores options whether from the CLH or from library user; initially valid only on worldRank = 0, but then broadcast in ParallelLibrary::push_output_tag() 

• struct partial_prp_hash
  wrapper to delegate to the ParamResponsePair hash_value function 

• struct partial_prp_equality
  predicate for comparing ONLY the interfaceId and Vars attributes of PRPair 

• class PSUADEDesignCompExp 
  Wrapper class for the PSUADE library. 

• class PythonInterface 

• class RandomFieldModel 
  Random field model, capable of generating and then forward propagating. 

• class RecastModel 
  Derived model class which provides a thin wrapper around a sub-model in order to recast the form of its inputs and/or outputs. 

• class ReducedBasis 

• class RelaxedVarConstraints 
  Derived class within the Constraints hierarchy which employs relaxation of discrete variables. 

• class RelaxedVariables 
  Derived class within the Variables hierarchy which employs the relaxation of discrete variables. 

• class ResultsDBAny 

• class ResultsID
  Get a globally unique 1-based execution number for a given iterator name (combination of methodName and methodID) for use in results DB. Each Iterator::run() call creates or increments this count for its string identifier. 

• class ResultsNames 
  List of valid names for iterator results. 

• class ResultsManager 
  Results manager for iterator final data. 

• class ResultsEntry 
  Class to manage in-core vs. file database lookups. 

• class RichExtrapVerification 
  Class for Richardson extrapolation for code and solution verification. 

• class ScalingModel 
  Scaling specialization of RecastModel. 

• class ScilabInterface 

• class SensAnalysisGlobal 
  Class for a utility class containing correlation calculations and variance-based decomposition. 

• class SeqHybridMetaIterator 
  Method for sequential hybrid iteration using multiple optimization and nonlinear least squares methods on multiple models of varying fidelity. 

• class SharedApproxData
CHAPTER 12. NAMESPACE DOCUMENTATION

Base class for the shared approximation data class hierarchy.

- class SharedPecosApproxData
  Derived approximation class for global basis polynomials.

- class SharedResponseDataRep
  The representation of a SharedResponseData instance. This representation, or body, may be shared by multiple SharedResponseData handle instances.

- class SharedResponseData
  Container class encapsulating variables data that can be shared among a set of Response instances.

- class SharedSurfpackApproxData
  Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

- class SharedVariablesDataRep
  The representation of a SharedVariablesData instance. This representation, or body, may be shared by multiple SharedVariablesData handle instances.

- class SharedVariablesData
  Container class encapsulating variables data that can be shared among a set of Variables instances.

- class SimulationModel
  Derived model class which utilizes a simulation-based application interface to map variables into responses.

- class SimulationResponse
  Container class for response functions and their derivatives. SimulationResponse provides the body class.

- class SNLLBase
  Base class for OPT++ optimization and least squares methods.

- class SNLLLeastSq
  Wrapper class for the OPT++ optimization library.

- class SNLLOptimizer
  Wrapper class for the OPT++ optimization library.

- class SOLBase
  Base class for Stanford SOL software.

- class SpawnApplicInterface
  Derived application interface class which spawns simulation codes using spawnvp.

- class SurfpackApproximation
  Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

- class SurrBasedGlobalMinimizer
  The global surrogate-based minimizer which sequentially minimizes and updates a global surrogate model without trust region controls.

- class SurrBasedLocalMinimizer
  Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

- class SurrBasedMinimizer
  Base class for local/global surrogate-based optimization/least squares.

- class SurrogateModel
  Base class for surrogate models (DataFitSurrModel and HierarchSurrModel).

- class SysCallApplicInterface
  Derived application interface class which spawns simulation codes using system calls.

- class TANA3Approximation
  Derived approximation class for TANA-3 two-point exponential approximation (a multipoint approximation).
• class **TaylorApproximation**
  
  *Derived approximation class for first- or second-order Taylor series (a local approximation).*

• class **TestDriverInterface**

• class **TrackerHTTP**
  
  *TrackerHTTP: a usage tracking module that uses HTTP/HTTPS via the curl library.*

• class **UsageTracker**
  
  *Lightweight class to manage conditionally active curl-based HTTP tracker via PIMPL.*

• class **VPSApproximation**
  
  *Derived approximation class for VPS implementation.*

• struct **MatchesWC**
  
  *Predicate that returns true when the passed path matches the wildcard with which it was configured. Currently supports * and ?.*

• class **WorkdirHelper**

**Typedefs**

• typedef double **Real**

• typedef std::string **String**

• typedef
  
  Teuchos::SerialDenseVector
  
  < int, Real > **RealVector**

• typedef
  
  Teuchos::SerialDenseMatrix
  
  < int, Real > **RealMatrix**

• typedef
  
  Teuchos::SerialSymDenseMatrix
  
  < int, Real > **RealSymMatrix**

• typedef
  
  Teuchos::SerialDenseVector
  
  < int, int > **IntVector**

• typedef
  
  Teuchos::SerialDenseMatrix
  
  < int, int > **IntMatrix**

• typedef std::deque< bool > **BoolDeque**

• typedef boost::dynamic_bitset
  
  < unsigned long > **BitArray**

• typedef std::vector< BoolDeque > **BoolDequeArray**

• typedef std::vector< Real > **RealArray**

• typedef std::vector< RealArray > **Real2DArray**

• typedef std::vector< int > **IntArray**

• typedef std::vector< IntArray > **Int2DArray**

• typedef std::vector< short > **ShortArray**

• typedef std::vector< unsigned short > **UShortArray**

• typedef std::vector< UShortArray > **UShort2DArray**

• typedef std::vector
  
  < UShort2DArray > **UShort3DArray**
typedef std::vector<size_t> SizetArray
typedef std::vector<SizetArray> Sizet2DArray
typedef std::vector<Sizet2DArray> Sizet3DArray
typedef std::vector<String> StringArray
typedef std::vector<StringArray> String2DArray
typedef boost::multi_array_types::index_range idx_range
typedef boost::multi_array
< String, 1 > StringMultiArray
typedef boost::multi_array
< String, 2 > StringMulti2DArray
typedef StringMultiArray::array_view
< 1 >::type StringMultiArrayView
typedef StringMultiArray::const_array_view
< 1 >::type StringMultiArrayConstView
typedef boost::multi_array
< unsigned short, 1 > UShortMultiArray
typedef UShortMultiArray::array_view
< 1 >::type UShortMultiArrayView
typedef UShortMultiArray::const_array_view
< 1 >::type UShortMultiArrayConstView
typedef boost::multi_array
< size_t, 1 > SizetMultiArray
typedef SizetMultiArray::array_view
< 1 >::type SizetMultiArrayView
typedef SizetMultiArray::const_array_view
< 1 >::type SizetMultiArrayConstView
typedef boost::multi_array
< Real, 1 > RealMultiArray
typedef boost::multi_array
< Real, 2 > RealMulti2DArray
typedef boost::multi_array
< Real, 3 > RealMulti3DArray
typedef std::vector<RealVector> RealVectorArray
typedef std::vector<RealVectorArray>
< RealVectorArray > RealVector2DArray
typedef std::vector<RealMatrix> RealMatrixArray
typedef std::vector<RealSymMatrix> RealSymMatrixArray
typedef std::vector<Variables> VariablesArray
typedef std::vector<Response> ResponseArray
12.1. DAKOTA NAMESPACE REFERENCE

- `typedef std::vector< ParamResponsePair > PRPArray`
- `typedef std::vector< PRPArray > PRP2DArray`
- `typedef std::vector< Model > ModelArray`
- `typedef std::vector< Iterator > IteratorArray`
- `typedef std::vector< RealMultiArray > BoostMAArray`
- `typedef std::vector< RealMulti2DArray > BoostMA2DArray`
- `typedef std::vector< RealMulti3DArray > BoostMA3DArray`
- `typedef std::list< bool > BoolList`
- `typedef std::list< int > IntList`
- `typedef std::list< size_t > SizetList`
- `typedef std::list< Real > RealList`
- `typedef std::list< RealVector > RealVectorList`
- `typedef std::list< String > StringList`
- `typedef std::list< Variables > VariablesList`
- `typedef std::list< Interface > InterfaceList`
- `typedef std::list< Response > ResponseList`
- `typedef std::list< ParamResponsePair > PRPList`
- `typedef std::list< Model > ModelList`
- `typedef std::list< Iterator > IteratorList`
- `typedef std::pair< int, int > IntIntPair`
- `typedef std::pair< size_t, size_t > SizetSizetPair`
- `typedef std::pair< SizetSizetPair, SizetSizetPair > SizetSizet2DPair`
- `typedef std::pair< size_t, int > SizetIntPair`
- `typedef std::pair< int, size_t > IntSizetPair`
- `typedef std::pair< int, String > IntStringPair`
- `typedef std::pair< Real, Real > RealRealPair`
- `typedef std::pair< int, Response > IntResponsePair`
- `typedef std::set< Real > RealSet`
- `typedef std::set< int > IntSet`
- `typedef std::set< String > StringSet`
- `typedef std::set< unsigned short > UShortSet`
- `typedef std::set< size_t > SizetSet`
- `typedef std::set< RealRealPair > RealRealPairSet`
- `typedef std::vector< RealSet > RealSetArray`
- `typedef std::vector< IntSet > IntSetArray`
- `typedef std::vector< StringSet > StringSetArray`
- `typedef std::vector< UShortSet > UShortSetArray`
- `typedef std::map< int, int > IntIntMap`
- `typedef std::map< int, short > IntShortMap`
- `typedef std::map< int, Real > IntRealMap`
• typedef std::map< Real, Real > RealRealMap
• typedef std::map< String, Real > StringRealMap
• typedef std::multimap< Real, int > RealIntMultiMap
• typedef std::vector< RealRealPair > RealRealPairArray
• typedef std::vector< IntRealMap > IntRealMapArray
• typedef std::vector< RealRealMap > RealRealMapArray
• typedef std::vector< StringRealMap > StringRealMapArray
• typedef std::map< Int, RealVector > IntRealVectorMap
• typedef std::map< Int, RealMatrix > IntRealMatrixMap
• typedef std::map< Int, ActiveSet > IntActiveSetMap
• typedef std::map< Int, Variables > IntVariablesMap
• typedef std::map< Int, Response > IntResponseMap
• typedef std::map< IntArray, size_t > IntArraySizetMap
• typedef std::map< IntIntPair, Real > IntIntPairRealMap
• typedef std::map< IntIntPair, RealMatrix > IntIntPairRealMatrixMap
• typedef std::map< RealRealPair, Real > RealRealPairRealMap
• typedef std::vector< IntIntPairRealMap > IntIntPairRealMapArray
• typedef std::vector< RealRealPairRealMap > RealRealPairRealMapArray
• typedef std::multimap< RealRealPair, ParamResponsePair > RealPairPRPMultiMap
• typedef std::map< SizetSizet2DPair, DiscrepancyCorrection > DiscrepCorrMap
• typedef IntlList::iterator ILIter
• typedef IntlList::const_iterator ILCIter
• typedef SizetList::iterator StLIter
• typedef SizetList::const_iterator StLCIter
• typedef RealList::iterator RLIter
• typedef RealList::const_iterator RLCIter
• typedef RealVectorList::iterator RVLIter
• typedef RealVectorList::const_iterator RVLCIter
• typedef StringList::iterator StringLIter
• typedef StringList::const_iterator StringLCIter
• typedef VariablesList::iterator VarsLIter
• typedef InterfaceList::iterator InterfLIter
• typedef ResponseList::iterator RespLIter
• typedef PRPList::iterator PRPLIter
• typedef ModelList::iterator ModelLIter
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- typedef ModelList::reverse_iterator ModelRevIter
- typedef IteratorList::iterator IterLIter
- typedef std::list<br>\texttt{< ParallelLevel >}::iterator ParLevLIter
- typedef std::list<br>\texttt{< ParallelConfiguration >}::iterator ParConfigLIter
- typedef IntSet::iterator ISIter
- typedef IntSet::const_iterator ISCIter
- typedef StringSet::iterator SSIter
- typedef StringSet::const_iterator SSCIter
- typedef RealSet::iterator RSIter
- typedef RealSet::const_iterator RSCIter
- typedef IntIntMap::iterator IntIntMIter
- typedef IntIntMap::const_iterator IntIntMCIter
- typedef IntShortMap::iterator IntShMIter
- typedef IntShortMap::const_iterator IntShMCIter
- typedef IntRealMap::iterator IRMIter
- typedef IntRealMap::const_iterator IRMCIter
- typedef StringRealMap::iterator SRMIter
- typedef StringRealMap::const_iterator SRMCIter
- typedef RealRealMap::iterator RRMIter
- typedef RealRealMap::const_iterator RRMCIter
- typedef IntIntPairRealMap::iterator IIPRMIter
- typedef IntIntPairRealMap::const_iterator IIPRMCIter
- typedef RealRealPairSet::iterator RRPSIter
- typedef RealRealPairSet::const_iterator RRPSCIter
- typedef RealRealPairRealMap::iterator RRPRMIter
- typedef RealRealPairRealMap::const_iterator RRPRMCIter
- typedef IntRealVectorMap::iterator IntRVMIter
- typedef IntRealVectorMap::const_iterator IntRVMCIter
- typedef IntRealMatrixMap::iterator IntRMMIter
- typedef IntRealMatrixMap::const_iterator IntRMMCIter
- typedef IntActiveSetMap::iterator IntASMIter
- typedef IntVariablesMap::iterator IntVarsIter
- typedef IntVariablesMap::const_iterator IntVarsMIter
- typedef IntResponseMap::iterator IntRespIter
- typedef IntResponseMap::const_iterator IntRespMIter
typedef boost::tuple
< std::string, std::string,
size_t, std::string > ResultsKeyType

Data type for results key (instance name / id, unique run, label), where data_key is a valid colon-delimited string
from ResultsNames tuple <method_name, method_id, execution_number, data_key>

typedef std::string MetaDataKeyType

Data type for metadata key.

typedef std::vector< std::string > MetaDataValueType

Data type for metadata value.

typedef std::map< MetaDataKeyType, MetaDataValueType > MetaDataType

A single MetaData entry is map <string, vector<string>> Example: pair("Column labels", ["Mean", "Std Dev", "Skewness", "Kurtosis"])

typedef boost::tuple
< std::string, std::string,
size_t > StrStrSizet

Iterator unique ID: <method_name, method_id, exec_num>

typedef void(* dl_core_run_t)(void *, Optimizer1 *, char *)

typedef void(* dl_destructor_t)(void **)

typedef Teuchos::SerialDenseSolver
< int, Real > RealSolver

typedef Teuchos::SerialSpdDenseSolver
< int, Real > RealSpdSolver

typedef int(* start_grid_computing_t)(char *analysis_driver_script, char *params_file, char *results_file)

definition of start grid computing type (function pointer)

typedef int(* perform_analysis_t)(char *, iteration_num)

definition of perform analysis type (function pointer)

typedef int (*)(* get_jobs_completed_t)()

definition of get completed jobs type (function pointer)

typedef int (*)(* stop_grid_computing_t)()

definition of stop grid computing type (function pointer)

typedef int MPI_Comm

typedef void * MPI_Request

typedef unsigned char u_char

typedef unsigned short u_short

typedef unsigned int u_int

typedef unsigned long u_long

typedef long long long_long

typedef unsigned long UL

typedef void(* Calcrj)(int *, int *, Real *, Real *, Real *, int *, void *, Vf, Vf *)

typedef void(* Vf)(*)

typedef void(* DbCallbackFunctionPtr)(Dakota::ProblemDescDB *db, void *data_ptr)
• typedef boost::tuple
  < bfs::path, bfs::path,
  bfs::path > PathTriple

  *Triplet of filesystem paths: e.g., params, results, workdir.*

• typedef bmi::multi_index_container
  < Dakota::ParamResponsePair,
  bmi::indexed_by
  < bmi::ordered_non_unique
  < bmi::tag< ordered >
  , bmi::const_mem_fun
  < Dakota::ParamResponsePair,
  const IntStringPair
  &,&Dakota::ParamResponsePair::eval_interface_ids >
  >, bmi::hashed_non_unique
  < bmi::tag< hashed >
  , bmi::identity
  < Dakota::ParamResponsePair>
  , partial_prp_hash,
  partial_prpequality > > > PRPMultiIndexCache

  *Boost Multi-Index Container for globally caching ParamResponsePairs.*

• typedef PRPMultiIndexCache PRPCache

• typedef PRPCache::index_iterator
  < ordered >::type PRPCacheOIter

• typedef PRPCache::index_const_iterator
  < ordered >::type PRPCacheOCIter

• typedef PRPCache::index_iterator
  < hashed >::type PRPCacheHIter

• typedef PRPCache::index_const_iterator
  < hashed >::type PRPCacheHCIter

• typedef PRPCache::index_iterator
  PRPCacheIter

  *default cache iterator <0>*

• typedef PRPCache::index_const_iterator
  PRPCacheIter

  *default cache const iterator <0>*

• typedef boost::reverse_iterator
  < PRPCacheIter > PRPCacheCRevIter

• typedef
bmi::multi_index_container
< Dakota::ParamResponsePair,
bmi::indexed_by
< bmi::ordered_unique
< bmi::tag< ordered >
, bmi::const_mem_fun
< Dakota::ParamResponsePair,
int,&Dakota::ParamResponsePair::eval_id >
>, bmi::hashed_non_unique
< bmi::tag< hashed >
, bmi::identity
< Dakota::ParamResponsePair >
, partial_prp_hash,
partial_prp_equality >> > > PRPMultiIndexQueue

 Boost Multi-Index Container for locally queueing ParamResponsePairs.

• typedef PRPMultiIndexQueue PRPQueue
• typedef
  PRPQueue::index_iterator
  < ordered >::type PRPQueueOIter
• typedef
  PRPQueue::index_const_iterator
  < ordered >::type PRPQueueOClIter
• typedef
  PRPQueue::index_iterator
  < hashed >::type PRPQueueHIter
• typedef
  PRPQueue::index_const_iterator
  < hashed >::type PRPQueueHCIter
• typedef PRPQueueOIter PRPQueueIter
• typedef PRPQueueOClIter PRPQueueCIter
• typedef
  std::pair< boost::any,
  MetaDataType > ResultsValueType

 Core data storage type: boost::any, with optional metadata (see other types in results_types.hpp)

• typedef boost::function< bool(const
bfs::path &src_path, const
bfs::path &dest_path, bool
overwrite)>
  file_op_function

 define a function type that operates from src to dest, with option to overwrite

• typedef boost::filter_iterator
  < MatchesWC,
bfs::directory_iterator >
  glob_iterator

 a glob_iterator filters a directory_iterator based on a wildcard predicate

Enumerations

• enum {
  COBYLA, DIRECT, EA, MS,
  PS, SW, BETA }


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- enum {
  METHOD_ERROR = -7, MODEL_ERROR = -6, IO_ERROR = -5, INTERFACE_ERROR = -4, 
  CONSTRUCT_ERROR = -3, PARSE_ERROR = -2, OTHER_ERROR = -1 
  }
  
  enum for Dakota abort reasons; using negative numbers to distinguish Dakota exit states from signals / uncaught 
  signals. These need to be in range [-63, -1], so exit code (256+enum) is in [193, 255]. See RATIONALE in 
  dakota_global_defs.cpp.

- enum { ABORT_EXITS, ABORT_THROWS }
  
  enum for dakota abort behaviors

- enum { CV_ID_DEFAULT = 0, MINIMUM_METRIC, RELATIVE_TOLERANCE, DECREASE_TOLERANCE }
  
  enum for active subspace cross validation identification

- enum {
  TABULAR_NONE = 0, TABULAR_HEADER = 1, TABULAR_EVAL_ID = 2, TABULAR_IFACE_ID = 4, 
  TABULAR_EXPER_ANOT = TABULAR_HEADER | TABULAR_EVAL_ID, TABULAR_ANOTATED = TABULAR_HEADER | TABULAR_EVAL_ID | TABULAR_IFACE_ID }
  
  options for tabular columns

- enum { FLEXIBLE_RESULTS, LABELED_RESULTS }
  
  options for results file format

- enum {
  NO_MODEL_FORMAT =0, TEXT_ARCHIVE =1, BINARY_ARCHIVE =2, ALGEBRAIC_FILE =4, 
  ALGEBRAIC_CONSOLE =8 }
  
  define special values for surrogateExportFormats

- enum {
  DEFAULT_INTERFACE =0, APPROX_INTERFACE, FORK_INTERFACE =PROCESS_INTERFACE, 
  SYSTEM_INTERFACE, GRID_INTERFACE, TEST_INTERFACE =DIRECT_INTERFACE, MATLAB_INTERFACE, PYTHON_INTERFACE, 
  SCILAB_INTERFACE }
  
  special values for interface type

- enum { SYNCHRONOUS_INTERFACE, ASYNCHRONOUS_INTERFACE }
  
  interface synchronization types

- enum { OBJECTIVE, INEQUALITY_CONSTRAINT, EQUALITY_CONSTRAINT }
  
  define algebraic function types

- enum {
  DEFAULT_METHOD =0, HYBRID =(META_BIT | PARALLEL_BIT), PARETO_SET, MULTI_START, 
  RICHARDSON_EXTRAP =(ANALYZER_BIT | VERIF_BIT), CENTERED_PARAMETER_STUDY 
  =(ANALYZER_BIT | PSTUDYDAUCE_BIT), LIST_PARAMETER_STUDY, MULTIDIM_PARAMETER_STUDY, 
  VECTOR_PARAMETER_STUDY, DACE, FSU_CVT, FSU_HALTON, 
  FSU_HAMMERSLEY, PSUADE_MOAT, LOCAL_RELIABILITY = (ANALYZER_BIT | NOND_BIT), 
  GLOBAL_RELIABILITY, POLYNOMIAL_CHAOS, STOCH_COLLOCATION, CUBATURE_INTEGRATION, SPARSE_GRID_INTEGRATION, 
  QUADRATURE_INTEGRATION, BAYES_CALIBRATION, GPAIS, POF_DARTS, 
  RKD_DARTS, IMPORTANCE_SAMPLING, ADAPTIVE_SAMPLING, MULTILEVEL_SAMPLI-
NG,
LIST_SAMPLING, RANDOM_SAMPLING, LOCAL_INTERVAL_EST, LOCAL_EVIDENCE,
GLOBAL_INTERVAL_EST, GLOBAL_EVIDENCE, SURROGATE_BASED_LOCAL = (MINIMIZER_BIT | SURRBASED_BIT), DATA_FIT_SURROGATE_BASED_LOCAL,
HIERARCH_SURROGATE_BASED_LOCAL, SURROGATE_BASED_GLOBAL, EFFICIENT_GLOBAL,
NL2SOL = (MINIMIZER_BIT | LEASTSQ_BIT),
NLSSOL_SQP, OPTPP_G_NEWTON, ASYNCH_PATTERN_SEARCH = (MINIMIZER_BIT | OPTIMIZER_BIT), OPTPP_PDS,
COLINY_BETA, COLINY_COBYLA, COLINY_DIRECT, COLINY_MULTI_START,
COLINY_EA, COLINY_PATTERN_SEARCH, COLINY_SOLIS_WETS, MOGA,
SOGA, NCSU_DIRECT, MESH_ADAPTIVE_SEARCH, MIT_NOWPAC,
MIT_SNOWPAC, GENIE_OPT_DARTS, GENIE_DIRECT, NONLINEAR.CG,
OPTPP.CG, OPTPP_Q_NEWTON, OPTPP_FD_NEWTON, OPTPP.NEWTON,
NPSOL_SQP, NLQL_SQP, DOT_BFGS, DOT_FRGC,
DOT_MMFD, DOT_SLP, DOT_SQP, CONMIN_FRGC,
CONMIN_MFD, DL_SOLVER/Branch_and_Bound = (MINIMIZER_BIT | OPTIMIZER_BIT | LEASTSQ_BIT))

• enum {
  SUBMETHOD_DEFAULT = 0, SUBMETHOD_NONE, SUBMETHOD_COLLABORATIVE, SUBMETHOD_EMBEDDED,
  SUBMETHODSEQUENTIAL, SUBMETHOD_LHS, SUBMETHODRANDOM, SUBMETHOD_BOX_BEHNKEN,
  SUBMETHOD_CENTRAL_COMPOSITE, SUBMETHOD_GRID, SUBMETHOD_OA_LHS, SUBMETHOD_OAS,
  SUBMETHOD_DREAM, SUBMETHOD_GPMSA, SUBMETHOD_QUESO, SUBMETHOD_WASABI,
  SUBMETHOD_NIP, SUBMETHOD_SQP, SUBMETHOD_EA, SUBMETHOD_EGO,
  SUBMETHOD_SBO, SUBMETHOD_CONVERGE_ORDER, SUBMETHOD_CONVERGE_QOI, SUBMETHOD_ESTIMATE_ORDER
}

  Sub-methods, including sampling, inference algorithm, opt algorithm types.

• enum {
  SILENT_OUTPUT, QUIET_OUTPUT, NORMAL_OUTPUT, VERBOSE_OUTPUT,
  DEBUG_OUTPUT
}

• enum {
  DEFAULT_SCHEDULING, MASTER_SCHEDULING, PEER_SCHEDULING, PEER_DYNAMIC_SCHEDULING,
  PEER_STATIC_SCHEDULING, DYNAMIC_SCHEDULING, STATIC_SCHEDULING
}

• enum {
  DEFAULT_CONFIG, PUSH_DOWN, PUSH_UP
}

• enum {
  STD_NORMAL_U, STD_UNIFORM_U, ASKEY_U, EXTENDED_U
}

• enum {
  DEFAULT_COVARIANCE, NO_COVARIANCE, DIAGONAL_COVARIANCE, FULL_COVARIANCE
}

• enum {
  NO_INT_REFINE = 0, IS, AIS, MMAIS
}

• enum {
  PROBABILITIES, RELIABILITIES, GEN_RELIABILITIES
}

• enum {
  COMPONENT = 0, SYSTEM_SERIES, SYSTEM_PARALLEL
}

• enum {
  CUMULATIVE, COMPLEMENTARY
}

• enum {
  NO_MOMENTS, STANDARD_MOMENTS, CENTRAL_MOMENTS
}

• enum {
  DEFAULT_LS = 0, SVD_LS, EQ_CON_LS
}
• enum {
    NO_EMULATOR, PCE_EMULATOR, SC_EMULATOR, GP_EMULATOR,
    KRINGING_EMULATOR, VPS_EMULATOR }

• enum {
    CALIBRATE_NONE = 0, CALIBRATE_ONE, CALIBRATE_PER_EXPER, CALIBRATE_PER_R-
    ESP, CALIBRATE_BOTH }

• enum { IGNORE_RANKS, SET_RANKS, GET_RANKS, SET_GET_RANKS }

• enum {
    UNCERTAIN, UNCERTAIN_UNIFORM, ALEATORY_UNCERTAIN, ALEATORY_UNCERTAI-
    N_UNIFORM, EPSTEERIC_UNCERTAIN, EPSTEERIC_UNCERTAIN_UNIFORM, ACTIVE, ACTIVE_UNIF-
    ORM, ALL, ALL_UNIFORM }

• enum { ONE_SIDED_LOWER, ONE_SIDED_UPPER, TWO_SIDED }

• enum {
    MV =0, AMV_X, AMV_U, AMV_PLUS_X, AMV_PLUS_U, TANA_X, TANA_U, NO_APPROX, 
    EGRA_X, EGRA_U }

• enum { BREITUNG, HOHENRACK, HONG }

• enum { ORIGINAL_PRIMARY, SINGLE_OBJECTIVE, LAGRANGIAN_OBJECTIVE, AUGME-
    NTED_LAGRANGIAN_OBJECTIVE }

• enum { NO_CONSTRAINTS, LINEARIZED_CONSTRAINTS, ORIGINAL_CONSTRAINTS }

• enum { NO_CONSTRAINTS, LINEARIZED_CONSTRAINTS, ORIGINAL_CONSTRAINTS }

• enum { PENALTY_MERIT, ADAPTIVE_PENALTY_MERIT, LAGRANGIAN_MERIT, AUGME-
    NTED_LAGRANGIAN_MERIT }

• enum { FILTER, TR_RATIO }

• enum { SCALE_NONE, SCALE_VALUE, SCALE_LOG }

• enum { CDV, LINEAR, NONLIN, FN_LSQ }

• enum { DISALLOW, TARGET_BOUNDS }

• enum { DEFAULT_POINTS, MINIMUM_POINTS, RECOMMENDED_POINTS, TOTAL_POINTS }

    define special values for pointsManagement

• enum {
    NO_SURROGATE =0, UNCORRECTED_SURROGATE, AUTO_CORRECTED_SURROGATE, B-
    YPASS_SURROGATE, MODEL_DISCREPANCY, AGGREGATED_MODELS }

    define special values for SurrogateModel::responseMode

• enum { NO_CORRECTION =0, ADDITIVE_CORRECTION, MULTIPlicative_CORRECTION, 
    COMBINED_CORRECTION }

    define special values for approxCorrectionType

• enum { RF_KARHUNEN_LOEVE =0, RF_PCA_GP, RF_ICA }

    define types of random field approximations

• enum { NOCOVAR =0, EXP_L2, EXP_L1 }

    define types of analytic covariance functions

• enum { SUBSPACE_NORM_DEFAULT =0, SUBSPACE_NORM_MEAN_VALUE, SUBSPACE_NO-
    RM_MEAN_GRAD, SUBSPACE_NORM_LOCAL_GRAD }
define special values for active subspace normalizations

- enum { SURROGATE_MODEL =1, TRUTH_MODEL }

define special values for componentParallelMode (active model for parallel scheduling)

- enum { BASE_RESPONSE =0, SIMULATION_RESPONSE, EXPERIMENT_RESPONSE }

special values for derived Response type

- enum { GENERIC_FNS = 0, OBJECTIVE_FNS, CALIB_TERMS }

values for primary response types

- enum { DEFAULT_DOMAIN =0, RELAXED_DOMAIN, MIXED_DOMAIN }

- enum {
  DEFAULT_VIEW =0, ALL_VIEW, DESIGN_VIEW, UNCERTAIN_VIEW,
  ALEATORY_UNCERTAIN_VIEW, EPISTEMIC_UNCERTAIN_VIEW, STATE_VIEW }

- enum {
  EMPTY_VIEW =0, RELaxed_ALL, MIXed_ALL, RELaxed_DEsign,
  RELaxed_UNcertain, RELaxed_Aleatory_UNcertain, RELaxed_EpiSTEMIC_UNcertain,
  RELaxed_STATE,
  MIXed_DEsign, MIXed_UNcertain, MIXed_Aleatory_UNcertain, MIXed_EpiSTEMIC_UNcertain,
  MIXed_STATE }

- enum { ALL_VARS =0, ACTIVE_VARS, INACTIVE_VARS }

values differentiating subsets of variables for I/O

- enum {
  EMPTY_TYPE =0, CONTINUOUS_DEsign, DISCRETE_DEsign_Range, DISCRETE_DEsign_SET_INt,
  DISCRETE_DEsign_SET_STRING, DISCRETE_DEsign_SET_REAL, NORMAL_UNcertain,
  LOGNORMAL_UNcertain,
  UNIFORM_UNcertain, LOGUNIFORM_UNcertain, TRIANGULAR_UNcertain, EXPONENTIAL_UNcertain,
  BETA_UNcertain, GAMMA_UNcertain, GUMBEL_UNcertain, FRECHET_UNcertain,
  WEIBULL_UNcertain, HISTOGRAM_BIN_UNcertain, POISSON_UNcertain, BINOMIAL_UNcertain,
  NEGATIVE_BINOMIAL_UNcertain, GEOMETRIC_UNcertain, HYPERGEOMETRIC_UNcertain,
  HISTOGRAM_POINT_UNcertain_INT,
  HISTOGRAM_POINT_UNcertain_STRING, HISTOGRAM_POINT_UNcertain_REAL, CONTINUOUS_INTERVAL_UNcertain,
  DISCRETE_INTERVAL_UNcertain, DISCRETE_UNcertain_SET_INT, DISCRETE_UNcertain_SET_STRING,
  DISCRETE_UNcertain_SET_REAL, CONTINUOUS_STATE,
  DISCRETE_STATE_RANGE, DISCRETE_STATE_SET_INT, DISCRETE_STATE_SET_STRING,
  DISCRETE_STATE_SET_REAL }

- enum {
  TOTAL_CDV =0, TOTAL_DDv, TOTAL_DSSV, TOTAL_DDRV,
  TOTAL_CAuv, TOTAL_DAuv, TOTAL_DAUv, TOTAL_DAURv,
  TOTAL_CEuv, TOTAL_DEuv, TOTAL_DEUSv, TOTAL_DEURv,
  TOTAL_CSv, TOTAL_DSIV, TOTAL_DSSV, TOTAL_DSRV,
  NUM_VC_TOTAls }

- enum var_t {
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VAR_x1, VAR_x2, VAR_x3, VAR_b,
VAR_h, VAR_P, VAR_M, VAR_Y,
VAR_w, VAR_t, VAR_R, VAR_E,
VAR_X, VAR_Fs, VAR_P1, VAR_P2,
VAR_P3, VAR_B, VAR_D, VAR_H,
VAR_F0, VAR_d, VAR_MForm

- enumeration of possible variable types (to index to names)
  - enum driver_t { NO_DRIVER = 0, CANTILEVER_BEAM, MOD_CANTILEVER_BEAM, CYLINDER_HEAD,
    EXTENDED_ROSENBOCK, GENERALIZED_ROSENBOCK, EXTRA_LF_ROSENBOCK,
    MF_ROSENBOCK, MODIFIED_ROSENBOCK, ROSENBOCK, LF_POLY_PROD,
    POLY_PROD, GERSTNER, SCALABLE, LOGNORMAL_RATIO,
    MULTIMODAL, PLUGIN_ROSENBOCK, PLUGIN_TEXT_BOOK, SHORT_COLUMN,
    MF_SHORT_COLUMN, MF_SHORT_COLUMN, SIDE_IMPACT_COST, SIDE_IMPACT_PERFORMANCE,
    SOBOL_RATIONAL, SOBOL_G_FUNCTION, STEEL_COLUMN_COST,
    STEEL_COLUMN_PERFORMANCE, TEXT_BOOK, TEXT_BOOK1, TEXT_BOOK2,
    TEXT_BOOK3, TEXT_BOOK_OUU, SCALABLE_TEXT_BOOK, SCALABLE_MONOMIALS,
    MOGATEST1, MOGATEST2, MOGATEST3, ILLUMINATION,
    BARNES, BARNES_LF, HERBIE, SMOOTH_HERBIE,
    SHUBERT, SALINAS, MODELCENTER, GENZ,
    DAMPED_OSCILLATOR, ANISOTROPIC_QUADRATIC_FORM, BAYES_LINEAR, STEADY_STATE_DIFFUSION_1D,
    TRANSIENT_DIFFUSION_1D, PREDATOR_PREY }
  - enumeration of possible direct driver types (to index to names)
  - enum local_data_t { VARIABLES_MAP = 1, VARIABLES_VECTOR = 2 }
    - enumeration for how local variables are stored (values must employ a bit representation)
  - enum sigtype { NO_SIGMA, SCALAR_SIGMA, DIAGONAL_SIGMA, MATRIX_SIGMA }
    - special values for sigmaType
  - enum edtype { SCALAR_DATA, FUNCTIONAL_DATA }
    - special values for experimental data type
  - enum { DEFAULT_CORRECTION = 0, SINGLE_CORRECTION, FULL_MODEL_FORM_CORRECTION,
    FULL_SOLUTION_LEVEL_CORRECTION, SEQUENCE_CORRECTION }
  - enum { SETUP_MODEL, SETUP_USERFUNC }
  - enum { CAUVar_normal = 0, CAUVar_lognormal = 1, CAUVar_uniform = 2, CAUVar_loguniform = 3,
    CAUVar_triangular = 4, CAUVar_exponential = 5, CAUVar_beta = 6, CAUVar_gamma = 7,
    CAUVar_gumbel = 8, CAUVar_frechet = 9, CAUVar_weibull = 10, CAUVar_histogram_bin = 11,
    CAUVar_Nkinds = 12 }
  - enum { DAUVar_poisson = 0, DAUVar_binomial = 1, DAUVar_negative_binomial = 2, DAUVar_geometric = 3,
    DAUVar_hypergeometric = 4, DAUVar_histogram_point_int = 5, DAUVar_Nkinds = 6 }
  - enum { DAUSVar_histogram_point_str = 0, DAUSVar_Nkinds = 1 }
  - enum { DAURVar_histogram_point_real = 0, DAURVar_Nkinds = 1 }
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- enum { CEUVar_interval = 0, CEUVar_Nkinds = 1 }
- enum { DEUIVar_interval = 0, DEUIVar_set_int = 1, DEUIVar_Nkinds = 2 }
- enum { DEUSVar_set_str = 0, DEUSVar_Nkinds = 1 }
- enum { DEURVar_set_real = 0, DEURVar_Nkinds = 1 }
- enum { DiscSetVar_design_set_int = 0, DiscSetVar_design_set_str = 1, DiscSetVar_design_set_real = 2, DiscSetVar_state_set_int = 3, DiscSetVar_state_set_str = 4, DiscSetVar_state_set_real = 5, DiscSetVar_Nkinds = 6 }
- enum { NUM_UNC_REAL_CONT = 4 } 
  number of real-valued uncertain contiguous containers
- enum { NUM_UNC_INT_CONT = 2 } 
  number of int-valued uncertain contiguous containers
- enum { NUM_UNC_STR_CONT = 2 } 
  number of string-valued uncertain contiguous containers
- enum { FULL_TENSOR, FILTERED_TENSOR, RANDOM_TENSOR }
- enum CG_UPDATETYPE { CG_STEEPEST, CG_FLETCHER_REEVES, CG_POLAK_RIBIERE, CG_POLAK_RIBIERE_PLUS, CGHESTENES_STIEFEL } 
  NonlinearCG update options.
- enum CG_LINESEARCHTYPE { CG_FIXED_STEP, CG_LS_SIMPLE, CG_LS_BRENT, CG_LS_WOLFE } 
  NonlinearCG linesearch options.
- enum EvalType { NLFEvaluator, CONEvaluator } 
  enumeration for the type of evaluator function
- enum { APPROX_RESPONSE =1, TRUTH_RESPONSE }
- enum { CORR_APPROX_RESPONSE =1, UNCORR_APPROX_RESPONSE, CORR_TRUTH_RESPONSE, UNCORR_TRUTH_RESPONSE }
- enum { NEW_CANDIDATE = 1, CANDIDATE_ACCEPTED = 2, CANDIDATE_STATE = (NEW_CANDIDATE | CANDIDATE_ACCEPTED), NEW_CENTER = 8, CENTER_BUILT = 16, CENTER_STATE = (NEW_CENTER | CENTER_BUILT), NEW_TR_FACTOR = 64, NEW_TRUST_REGION = (NEW_CENTER | NEW_TR_FACTOR), HARD_CONVERGED = 128, SOFT_CONVERGED = 256, MIN_TR_CONVERGED = 512, MAX_ITER_CONVERGED = 1024, CONVERGED }
- enum { TH_SILENT_OUTPUT, TH_QUIET_OUTPUT, TH_NORMAL_OUTPUT, TH_VERBOSE_OUTPUT, TH_DEBUG_OUTPUT }
- enum { DIR_CLEAN, DIR_PERSIST, DIR_ERROR } 
  define directory creation options
- enum { FILEOP_SILENT, FILEOP_WARN, FILEOP_ERROR } 
  enum indicating action on failed file operation
12.1. DAKOTA NAMESPACE REFERENCE

Functions

- CommandShell & flush (CommandShell &shell)
  convenient shell manipulator function to "flush" the shell
- void read_sized_data (std::istream &s, RealVectorArray &va, size_t num_rows, int num_cols)
- void read_fixed_rowsize_data (std::istream &s, RealVectorArray &va, int num_cols, bool row_major)
- void read_unsized_data (std::istream &s, RealVectorArray &va, bool row_major)
- void read_config_vars_multifile (const std::string &basename, int num_expts, int ncv, RealVectorArray &config_vars)
- void read_config_vars_singlefile (const std::string &basename, int num_expts, int ncv, RealVectorArray &config_vars)
- void read_field_values (const std::string &basename, int expt_num, RealVectorArray &field_vars)
- void read_field_values (const std::string &basename, int expt_num, RealVector &field_vars)
- void read_coord_values (const std::string &basename, int expt_num, RealMatrix &coords)
- void read_coord_values (const std::string &basename, RealMatrix &coords)
- void read_covariance (const std::string &basename, int expt_num, Dakota::CovarianceMatrix::FORMAT format, int num_vals, RealMatrix &cov_vals)
- void read_covariance (const std::string &basename, int expt_num, Dakota::CovarianceMatrix::FORMAT format, int num_vals, Dakota::CovarianceMatrix::FORMAT format, int num_vals, RealMatrix &cov_vals, RealMatrix &cov_vals)
- bool nearby (const RealVector &rv1, const RealVector &rv2, Real rel_tol)
  tolerance-based equality operator for RealVector
- bool operator== (const ShortArray &dsa1, const ShortArray &dsa2)
  equality operator for ShortArray
- bool operator== (const StringArray &dsa1, const StringArray &dsa2)
  equality operator for StringArray
- Real rel_change_L2 (const RealVector &curr(rv, const RealVector &prev(rv)
  Computes relative change between RealVectors using Euclidean L2 norm.
- Real rel_change_L2 (const RealVector &curr(rv1, const RealVector &prev(rv1, const IntVector &curr(iv),
  const IntVector &prev(iv), const RealVector &curr(rv2, const RealVector &prev(rv2)
  Computes relative change between Real/int/Real vector triples using Euclidean L2 norm.
- void remove_column (RealMatrix &matrix, int index)
  Removes column from matrix.
- void iround (const RealVector &input_vec, IntVector &rounded_vec)
  round entries of a RealVector yielding an IntVector
- bool operator== (const IntArray &dia1, const IntArray &dia2)
  equality operator for IntArray
- template<typename T>
  bool operator== (const std::vector<T> &vec, typename boost::multi_array<T, 1>::template const_array_view<1>::type mav)
  equality operator for std::vector and boost::multi_array::const_array_view
- template<typename T>
  bool operator== (typename boost::multi_array<T, 1>::template const_array_view<1>::type mav, const std::vector<T> &vec)
  equality operator for boost::multi_array::const_array_view and std::vector
- template<typename T>
  bool operator== (const boost::multi_array<T, 1> &ma, typename boost::multi_array<T, 1>::template const_array_view<1>::type mav)
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equality operator for boost::multi_array and boost::multi_array::const_array_view

- template<typename T>
  bool operator== (typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav, const boost::multi_array< T, 1 >&ma)

inequality operator for boost::multi_array::const_array_view and boost::multi_array

- bool operator!= (const IntArray &dia1, const IntArray &dia2)

inequality operator for IntArray

- bool operator!= (const ShortArray &dsa1, const ShortArray &dsa2)

inequality operator for ShortArray

- bool operator!= (const StringArray &dsa1, const StringArray &dsa2)

inequality operator for StringArray

- template<typename T>
  bool operator!= (const std::vector< T >&vec, typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav)

inequality operator for std::vector and boost::multi_array::const_array_view

- template<typename T>
  bool operator!= (typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav, const std::vector< T >&vec)

inequality operator for boost::multi_array::const_array_view and std::vector

- template<typename T>
  bool operator!= (const boost::multi_array< T, 1 >&ma, typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav)

inequality operator for boost::multi_array and boost::multi_array::const_array_view

- template<typename T>
  bool operator!= (typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav, const boost::multi_array< T, 1 >&ma)

inequality operator for boost::multi_array::const_array_view and boost::multi_array

- std::string strtolower (const std::string &s)
  Return lowercase copy of string s.

- bool strbegins (const std::string &input, const std::string &test)
  Return true if input string begins with string test.

- bool strends (const std::string &input, const std::string &test)
  Return true if input string ends with string test.

- bool strcontains (const std::string &input, const std::string &test)
  Return true if input string contains string test.

- void build_label (String &label, const String &root_label, size_t tag, const String &separator="")
  create a label by appending a numerical tag to the root_label, o

- void build_labels (StringArray &label_array, const String &root_label)
  create an array of labels by tagging root_label for each entry in label_array. Uses build_label().

- void build_labels (StringMultiArray &label_array, const String &root_label)
  create an array of labels by tagging root_label for each entry in label_array. Uses build_label().

- void build_labels_partial (StringArray &label_array, const String &root_label, size_t start_index, size_t num_items)
  create a partial array of labels by tagging root_label for a subset of entries in label_array. Uses build_label().
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- template<typename OrdinalType, typename ScalarType>
  void copy_data (const std::vector<Teuchos::SerialDenseVector<OrdinalType, ScalarType> > &sdva, Teuchos::SerialDenseMatrix<OrdinalType, ScalarType> &sdm)

    copy Array<Teuchos::SerialDenseVector<OT,ST> > to Teuchos::SerialDenseMatrix<OT,ST> - used by read_data_tabular - RWH

- template<typename OrdinalType, typename ScalarType>
  void copy_data_transpose (const std::vector<Teuchos::SerialDenseVector<OrdinalType, ScalarType> > &sdva, Teuchos::SerialDenseMatrix<OrdinalType, ScalarType> &sdm)

    copy Array<Teuchos::SerialDenseVector<OT,ST> > to transposed Teuchos::SerialDenseMatrix<OT,ST> - used by read_data_tabular - RWH

- template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data (const Teuchos::SerialDenseVector<OrdinalType1, ScalarType> &sdv, Teuchos::SerialDenseMatrix<OrdinalType1, ScalarType> &sdm, OrdinalType2 nr, OrdinalType2 nc)

    copy Teuchos::SerialDenseVector<OT,ST> to Teuchos::SerialDenseMatrix<OT,ST> - used by NestedModel::update_sub_iterator - RWH

- template<typename T>
  void copy_data (const std::vector<std::vector<T> > &d2a, std::vector<T> &da)

    copy std::vector<vector<T> > to std::vector<T>(unroll vecOfvecs into vector) - used by ProcessApplicInterface::write_parameters_files - RWH

- template<typename T>
  void copy_data (const std::map<int, T> &im, std::vector<T> &da)

    copy map<int, T> to std::vector<T>(discard integer keys) - used by SurrBasedGlobalMinimizer::core_run - RWH

- template<typename OrdinalType, typename ScalarType>
  void copy_data (const Teuchos::SerialDenseVector<OrdinalType, ScalarType> &sdv1, Teuchos::SerialDenseVector<OrdinalType, ScalarType> &sdv2)

    copy Teuchos::SerialDenseVector<OrdinalType, ScalarType> to same (used in place of operator= when a deep copy of a vector view is needed) - used by SensAnalysisGlobal::valid_sample_matrix - RWH

- template<typename OrdinalType, typename ScalarType, typename VectorType>
  void copy_data (const Teuchos::SerialDenseVector<OrdinalType, ScalarType> &sdv, VectorType &vec)

    copy Teuchos::SerialDenseVector<OrdinalType, ScalarType> to std::vector<ScalarType> - used by SurfpackApproximation constructor - RWH

- template<typename OrdinalType, typename ScalarType>
  void copy_data (const std::vector<ScalarType> &da, Teuchos::SerialDenseVector<OrdinalType, ScalarType> &sdv)

    copy Array<ScalarType> to Teuchos::SerialDenseVector<ScalarType> - used by NOWPACOptimizer - MSE

- template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data (const ScalarType *ptr, const OrdinalType2 ptr_len, Teuchos::SerialDenseVector<OrdinalType1, ScalarType> &sdv)

    copy ScalarType* to Teuchos::SerialDenseVector<OrdinalType, ScalarType> - used by ScalingModel::response_modify_p2s - RWH

- template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data (const Teuchos::SerialDenseVector<OrdinalType1, ScalarType> &sdv, ScalarType *ptr, const OrdinalType2 ptr_len)

    copy ScalarType* to Teuchos::SerialDenseVector<OrdinalType, ScalarType> - used by NL2SOLLeastSq::core_run - RWH
• template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data (const Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv, std::vector<Teuchos::SerialDenseVector<OrdinalType1, ScalarType>>& sdva, OrdinalType2 num_vec, OrdinalType2 vec_len)

  copy SerialDenseVector<> to Array<SerialDenseVector<> > - used by ConcurrentMetaIterator constructor - RWH

• template<typename vecType1, typename vecType2>
  void copy_data_partial (const vecType1 &source, vecType2 &target, size_t start_idx, size_t len)

  copy a portion arbitrary vector to all of another arbitrary vector

• template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data_partial (const Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv1, OrdinalType2 start_index1, OrdinalType2 num_items, Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv2)

  copy portion of first SerialDenseVector to all of second SerialDenseVector - used by DataTransformModel::vars_mapping - RWH

• template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data_partial (const Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv1, Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv2, OrdinalType2 start_index2)

  copy all of first SerialDenseVector to portion of second SerialDenseVector - used by MixedVariables - RWH

• template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data_partial (const Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv1, Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv2, OrdinalType2 start_index2)

  copy portion of first SerialDenseVector to portion of second SerialDenseVector - used by ScalingModel::secondary_resp_scaled2native - RWH

• template<typename OrdinalType1, typename OrdinalType2, typename ScalarType>
  void copy_data_partial (const Teuchos::SerialDenseVector<OrdinalType1, ScalarType>& sdv1, std::vector<ScalarType>& da2, OrdinalType2 start_index2)

  copy all of first SerialDenseVector to portion of second SerialDenseVector - used by SharedSurfpackApproxData::merge_variable_arrays - RWH

• template<typename T>
  void copy_data_partial (const std::vector<T>& da1, size_t start_index1, size_t num_items, std::vector<T>& da2)

  copy portion of first Array<T> to all of second Array<T> - used by SharedResponseDataRep constructor - RWH

• template<typename T>
  void copy_data_partial (const std::vector<T>& da1, std::vector<T>& da2, size_t start_index2)

  copy all of first Array<T> to portion of second Array<T> - used by ParamStudy::multidim_loop - RWH

• template<typename T>
  void copy_data_partial (const std::vector<T>& da, boost::multi_array<T, 1>& bma, size_t start_index, bma)

  copy all of first Array<T> to portion of boost::multi_array<T, 1> - used by RelaxedVariables - RWH

• template<typename VectorType>
  void copy_row_vector (const RealMatrix &m, RealMatrix::ordinalType i, VectorType &row)

  Copies a row of a Teuchos::SerialDenseMatrix<int, Real> to std::vector<Real>

• template<typename ScalarType>
  void insert_row_vector (const std::vector< ScalarType > &row, RealMatrix::ordinalType i, RealMatrix &m)
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Copies a row of a Teuchos_SerialDenseMatrix<int,Real> to std::vector<Real>

- void merge_data_partial (const IntVector &d_vec, RealVector &m_vec, size_t start_index_ma)
  merge a discrete integer vector into a single continuous vector

- void merge_data_partial (const IntVector &d_vec, RealArray &m_array, size_t start_index_ma)
  merge a discrete integer vector into a single continuous array

- template<typename OrdinalType , typename ScalarType >
  const ScalarType & set_index_to_value (OrdinalType index, const std::set<ScalarType> &values)
  retrieve the set value corresponding to the passed index

- template<typename ScalarType >
  size_t set_value_to_index (const ScalarType &value, const std::set<ScalarType> &values)
  calculate the set index corresponding to the passed value

- template<typename OrdinalType , typename KeyType , typename ValueType >
  const KeyType & map_index_to_key (OrdinalType index, const std::map<KeyType, ValueType> &pairs)
  retrieve the set value corresponding to the passed index

- template<typename OrdinalType , typename KeyType , typename ValueType >
  const ValueType & map_index_to_value (OrdinalType index, const std::map<KeyType, ValueType> &pairs)
  retrieve the set value corresponding to the passed index

- template<typename KeyType , typename ValueType >
  size_t map_key_to_index (const KeyType &key, const std::map<KeyType, ValueType> &pairs)
  calculate the map index corresponding to the passed key

- template<typename ContainerType >
  size_t find_index (const ContainerType &c, const typename ContainerType::value_type &search_data)
  generic find_index (inactive)

- template<typename T >
  size_t find_index (const boost::multi_array<T, 1> &bma, const T &search_data)
  compute the index of an entry within a boost::multi_array

- size_t find_index (SizetMultiArrayConstView bmacv, size_t search_data)
  compute the index of an entry within a boost::multi_array view

- size_t find_index (StringMultiArrayConstView bmacv, const String &search_data)
  compute the index of an entry within a boost::multi_array view

- template<typename ListT >
  size_t find_index (const ListT &l, const typename ListT::value_type &val)
  compute the index of an entry within a std::list

- template<typename ListT >
  ListT::const_iterator find_if (const ListT &c, bool(*test_fn)(const typename ListT::value_type &, const std::string &), const std::string &test_fn_data)
return an iterator to the first list element satisfying the predicate test_fn w.r.t. the passed test_fn_data; end if not found

- template<typename VectorType, typename ScalarType>
  void copy_data (const std::vector<VectorType> &va, ScalarType *ptr, int ptr_len)

- void copy_data (SizetMultiArrayConstView ma, SizetArray &da)
  copy boost::multi_array view to Array - used by ActiveSet::derivative_vector - RWH

- void copy_data (StringMultiArrayConstView ma, StringArray &da)
  copy boost::multi_array view to Array - used by Pecos::copy_data - RWH

- template<typename DakContainerType>
  bool contains (const DakContainerType &v, const typename DakContainerType::value_type &val)
  return true if the item val appears in container v

- void abort_handler (int code)
  global function which handles serial or parallel aborts

- void abort_throw_or_exit (int dakota_code)
  throw or exit depending on abort_mode

- void register_signal_handlers ()
  Tie various signal handlers to Dakota's abort_handler function.

- void mpi_debug_hold ()
  Global function to hold Dakota processes to help with MPI debugging.

- template<typename T>
  T abort_handler_t (int code)

- void svd (RealMatrix &matrix, RealVector &singular(vals, RealMatrix &v_trans, bool compute_vectors=true)
  Compute the SVD of an arbitrary matrix A = USV^T.

- void singular_values (RealMatrix &matrix, RealVector &singular(values)
  compute the singular values without storing any singular vectors (A will be destroyed)

- int qr (RealMatrix &A)
  Compute an in-place QR factorization A = QR.

- int qr_rsolve (const RealMatrix &q_r, bool transpose, RealMatrix &rhs)
  Perform a multiple right-hand sides Rinv * rhs solve using the R from a qr factorization.

- double det_AtransA (RealMatrix &A)
  Use SVD to compute det(A'*A), destroying A with the SVD.

- ResultsKeyType make_key (const StrStrSizet &iterator_id, const std::string &data_name)
  Make a full ResultsKeyType from the passed iterator_id and data_name.

-MetaDataValueType make_metadatavalue (StringMultiArrayConstView labels)
  create MetaDataValueType from the passed strings

-MetaDataValueType make_metadatavalue (StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels)
  create MetaDataValueType from the passed strings

-MetaDataValueType make_metadatavalue (const StringArray &resp_labels)
  create MetaDataValueType from the passed strings

-MetaDataValueType make_metadatavalue (const std::string &)
  create MetaDataValueType from the passed strings

-MetaDataValueType make_metadatavalue (const std::string &, const std::string &)
  create MetaDataValueType from the passed strings
• `MetaDataValueType make_metadatavalue` (const std::string &, const std::string &, const std::string &)
  create MetaDataValueType from the passed strings

• `MetaDataValueType make_metadatavalue` (const std::string &, const std::string &, const std::string &)
  create MetaDataValueType from the passed strings

• `MetaDataValueType make_metadatavalue` (StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView dsv_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels)

• `std::istream & operator>>(std::istream &s, ActiveSet &set)`
  std::istream extraction operator for ActiveSet. Calls read(std::istream&).

• `std::ostream & operator<<(std::ostream &s, const ActiveSet &set)`
  std::ostream insertion operator for ActiveSet. Calls write(std::istream&).

• `MPIUnpackBuffer & operator>>(MPIUnpackBuffer &s, ActiveSet &set)`
  MPIUnpackBuffer extraction operator for ActiveSet. Calls read(MPIUnpackBuffer&).

• `MPIPackBuffer & operator<<(MPIPackBuffer &s, const ActiveSet &set)`
  MPIPackBuffer insertion operator for ActiveSet. Calls write(MPIPackBuffer&).

• bool `operator!=(const ActiveSet &set1, const ActiveSet &set2)`
  inequality operator for ActiveSet

• `std::istream & operator>>(std::istream &s, Constraints &con)`
  std::istream extraction operator for Constraints

• `std::ostream & operator<<(std::ostream &s, const Constraints &con)`
  std::ostream insertion operator for Constraints

• `std::string re_match(const std::string &token, const boost::regex &re)`
  Global utility function to ease migration from CtelRegExp to Boost.Regex.

• bool `interface_id_compare(const Interface &interface_in, const void *id)`
  global comparison function for Interface

• bool `method_id_compare(const Iterator &iterator, const void *id)`
  global comparison function for Iterator

• bool `model_id_compare(const Model &model, const void *id)`
  global comparison function for Model

• bool `operator==(const Model &m1, const Model &m2)`
  equality operator for Envelope is true if same letter instance

• bool `operator!=(const Model &m1, const Model &m2)`
  inequality operator for Envelope is true if different letter instance

• `template< typename VectorType1 , typename VectorType2 , typename SetArray >
void copy_data(const VectorType1 &source, const BitArray &set_bits, const SetArray &set_vars, VectorType2 &dest, size_t offset, size_t len)`

• `template< typename VectorType1 , typename VectorType2 , typename SetArray >
void copy_data(const VectorType1 &source, const SetArray &set_vars, VectorType2 &dest, size_t offset, size_t len)`

• `template< typename VectorType1 , typename VectorType2 >
void copy_data(const VectorType1 &source, VectorType2 &dest, const BitArray &int_set_bits, const IntSetArray &int_set_vars, size_t offset, size_t len)`
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- template<typename AdapterT >
  void set_best_responses (typename AdapterT::OptT &optimizer, const Model &model, const std::vector<int> &constraintMapIndices, const std::vector<double> &constraintMapMultipliers, const std::vector<double> &constraintMapOffsets, ResponseArray &response_array)

  Data adapter for use by third-party opt packages to transfer response data to Dakota.

- template<typename VectorType >
  void set_variables (const VectorType &source, Model &model, Variables &vars)

  copy appropriate slices of source vector to Dakota::Variables

- template<typename VectorType >
  void get_variables (Model &model, VectorType &vec)

  copy the various pieces comprising Dakota::Variables into a concatenated TPL vector

- template<typename OrdinalType , typename ScalarType , typename VectorType2 , typename MaskType , typename SetArray >
  bool get_mixed_bounds (const MaskType &mask_set, const SetArray &source_set, const Teuchos::SerialDenseVector<OrdinalType, ScalarType> &lower_source, const Teuchos::SerialDenseVector<OrdinalType, ScalarType> &upper_source, VectorType2 &lower_target, VectorType2 &upper_target, ScalarType bigBoundSize, ScalarType no_value, int target_offset=0)

- template<typename OrdinalType , typename ScalarType , typename VectorType2 >
  bool get_bounds (const Teuchos::SerialDenseVector<OrdinalType, ScalarType> &lower_source, const Teuchos::SerialDenseVector<OrdinalType, ScalarType> &upper_source, VectorType2 &lower_target, VectorType2 &upper_target, ScalarType bigBoundSize, ScalarType no_value, int target_offset=0)

- template<typename SetArray , typename VectorType >
  void get_bounds (const SetArray &source_set, VectorType &lower_target, VectorType &upper_target, int target_offset=0)

- template<typename vectorType >
  void get_responses (const Model &model, const RealVector &dak_fn vals, const std::vector<int> &constraintMapIndices, const std::vector<double> &constraintMapMultipliers, const std::vector<double> &constraintMapOffsets, vectorType &f_vec, vectorType &cEqs_vec, vectorType &cIneqs_vec)

  Data adapter to transfer data from Dakota to third-party opt packages.

- template<typename AdapterT >
  bool get_bounds (Model &model, Real bigRealBoundSize, int bigIntBoundSize, typename AdapterT::VecT &lower, typename AdapterT::VecT &upper)

  copy the various pieces comprising bounds on Dakota::Variables into concatenated TPL vectors

- template<typename AdapterT >
  void get_linear_constraints (Model &model, Real bigRealBoundSize, typename AdapterT::VecT &lin_ineq_lower_bnds, typename AdapterT::VecT &lin_ineq_upper_bnds, typename AdapterT::VecT &lin_eq_targets, typename AdapterT::MatT &lin_ineq_coeffs, typename AdapterT::MatT &lin_eq_coeffs)

  copy the various data associated with linear constraints from Dakota into TPL vectors/matrices

- bool responses_id_compare (const Response &resp, const void *id)

  global comparison function for Response

- std::istream & operator>>(std::istream &s, Response &response)

  std::istream extraction operator for Response. Calls read(std::istream&).

- std::ostream & operator<<(std::ostream &s, const Response &response)

  std::ostream insertion operator for Response. Calls write(std::ostream&).

- MPIUnpackBuffer & operator>>(MPIUnpackBuffer &s, Response &response)

  MPIUnpackBuffer extraction operator for Response. Calls read(MPIUnpackBuffer&).

- MPIPackBuffer & operator<<(MPIPackBuffer &s, const Response &response)
MPIPackBuffer insertion operator for Response. Calls write(MPIPackBuffer&).

- bool operator!=(const Response &resp1, const Response &resp2)
  inequality operator for Response
- bool variables_id_compare(const Variables &vars, const void *id)
  global comparison function for Variables
- std::istream & operator>>(std::istream &, Variables &vars)
  std::istream extraction operator for Variables.
- std::ostream & operator<<(std::ostream &, const Variables &vars)
  std::ostream insertion operator for Variables.
- MPIUnpackBuffer & operator>>(MPIUnpackBuffer &, Variables &vars)
  MPIUnpackBuffer extraction operator for Variables.
- MPIPackBuffer & operator<<(MPIPackBuffer &, const Variables &vars)
  MPIPackBuffer insertion operator for Variables.
- bool operator!=(const Variables &vars1, const Variables &vars2)
  inequality operator for Variables
- template<typename OrdinalType, typename ScalarType1, typename ScalarType2, typename ScalarType3, typename ScalarType4>
  void write_ordered(std::ostream &, const SizetArray &comp_totals, const Teuchos::SerialDenseVector<OrdinalType, ScalarType1> &c_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType2> &d1_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType3> &d2_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType4> &d3_vector)
  free function to write Variables data vectors in input spec ordering
- template<typename OrdinalType, typename ScalarType1, typename ScalarType2, typename ScalarType3, typename ScalarType4>
  void write_ordered(std::ostream &, const SizetArray &comp_totals, const Teuchos::SerialDenseVector<OrdinalType, ScalarType1> &c_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType2> &d1_vector, const boost::multi_array<ScalarType3, 1> &d2_array, const Teuchos::SerialDenseVector<OrdinalType, ScalarType4> &d3_vector)
  free function to write Variables data vectors in input spec ordering
- template<typename ScalarType>
  void write_ordered(std::ostream &, const SizetArray &comp_totals, const std::vector<ScalarType> &c_array, const std::vector<ScalarType> &d1_array, const std::vector<ScalarType> &d2_array, const std::vector<ScalarType> &d3_array)
  free function to write Variables data vectors in input spec ordering
- MPIPackBuffer & operator<<(MPIPackBuffer &, const DataEnvironment &data)
  MPIPackBuffer insertion operator for DataEnvironment.
- MPIUnpackBuffer & operator>>(MPIUnpackBuffer &, DataEnvironment &data)
  MPIUnpackBuffer extraction operator for DataEnvironment.
- std::ostream & operator<<(std::ostream &, const DataEnvironment &data)
  std::ostream insertion operator for DataEnvironment
- String interface_enum_to_string(unsigned short interface_type)
- MPIPackBuffer & operator<<(MPIPackBuffer &, const DataInterface &data)
  MPIPackBuffer insertion operator for DataInterface.
- MPIUnpackBuffer & operator>>(MPIUnpackBuffer &, DataInterface &data)
  MPIUnpackBuffer extraction operator for DataInterface.
• \( \text{std::ostream} \& \text{operator} << \text{(std::ostream} \& s, \text{const DataInterface} \& \text{data}) \)

\( \text{std::ostream} \) insertion operator for DataInterface.

• \( \text{MPIPackBuffer} \& \text{operator} << \text{(MPIPackBuffer} \& s, \text{const DataMethod} \& \text{data}) \)

\( \text{MPIPackBuffer} \) insertion operator for DataMethod.

• \( \text{MPIUnpackBuffer} \& \text{operator} >> \text{(MPIUnpackBuffer} \& s, \text{DataMethod} \& \text{data}) \)

\( \text{MPIUnpackBuffer} \) extraction operator for DataMethod.

• \( \text{std::ostream} \& \text{operator} << \text{(std::ostream} \& s, \text{const DataMethod} \& \text{data}) \)

\( \text{std::ostream} \) insertion operator for DataMethod.

• \( \text{MPIPackBuffer} \& \text{operator} << \text{(MPIPackBuffer} \& s, \text{const DataModel} \& \text{data}) \)

\( \text{MPIPackBuffer} \) insertion operator for DataModel.

• \( \text{MPIUnpackBuffer} \& \text{operator} >> \text{(MPIUnpackBuffer} \& s, \text{DataModel} \& \text{data}) \)

\( \text{MPIUnpackBuffer} \) extraction operator for DataModel.

• \( \text{std::ostream} \& \text{operator} << \text{(std::ostream} \& s, \text{const DataModel} \& \text{data}) \)

\( \text{std::ostream} \) insertion operator for DataModel.

• \( \text{MPIPackBuffer} \& \text{operator} << \text{(MPIPackBuffer} \& s, \text{const DataResponses} \& \text{data}) \)

\( \text{MPIPackBuffer} \) insertion operator for DataResponses.

• \( \text{MPIUnpackBuffer} \& \text{operator} >> \text{(MPIUnpackBuffer} \& s, \text{DataResponses} \& \text{data}) \)

\( \text{MPIUnpackBuffer} \) extraction operator for DataResponses.

• \( \text{std::ostream} \& \text{operator} << \text{(std::ostream} \& s, \text{const DataResponses} \& \text{data}) \)

\( \text{std::ostream} \) insertion operator for DataResponses.

• \( \text{MPIPackBuffer} \& \text{operator} << \text{(MPIPackBuffer} \& s, \text{const DataVariables} \& \text{data}) \)

\( \text{MPIPackBuffer} \) insertion operator for DataVariables.

• \( \text{MPIUnpackBuffer} \& \text{operator} >> \text{(MPIUnpackBuffer} \& s, \text{DataVariables} \& \text{data}) \)

\( \text{MPIUnpackBuffer} \) extraction operator for DataVariables.

• \( \text{std::ostream} \& \text{operator} << \text{(std::ostream} \& s, \text{const DataVariables} \& \text{data}) \)

\( \text{std::ostream} \) insertion operator for DataVariables.

• int \( \text{dlsolver_option} \) (Opt_Info *)

• RealVector const * \( \text{continuous_lower_bounds} \) (Optimizer1 *o)

• RealVector const * \( \text{continuous_upper_bounds} \) (Optimizer1 *o)

• RealVector const * \( \text{nonlinear_ineq_constraint_lower_bounds} \) (Optimizer1 *o)

• RealVector const * \( \text{nonlinear_ineq_constraint_upper_bounds} \) (Optimizer1 *o)

• RealVector const * \( \text{nonlinear_eq_constraint_targets} \) (Optimizer1 *o)

• RealVector const * \( \text{linear_ineq_constraint_lower_bounds} \) (Optimizer1 *o)

• RealVector const * \( \text{linear_ineq_constraint_upper_bounds} \) (Optimizer1 *o)

• RealVector const * \( \text{linear_eq_constraint_targets} \) (Optimizer1 *o)

• RealMatrix const * \( \text{linear_ineq_constraint_coeffs} \) (Optimizer1 *o)

• RealMatrix const * \( \text{linear_eq_constraint_coeffs} \) (Optimizer1 *o)

• void \( \text{ComputeResponses} \) (Optimizer1 *o, int mode, int n, double *x)

• void \( \text{GetFuncs} \) (Optimizer1 *o, int m0, int m1, double *f)

• void \( \text{GetGrads} \) (Optimizer1 *o, int m0, int m1, int n, int is, int js, double *g)

• void \( \text{GetContVars} \) (Optimizer1 *o, int n, double *x)

• void \( \text{SetBestContVars} \) (Optimizer1 *o, int n, double *x)

• void \( \text{SetBestResps} \) (Optimizer1 *o, int n, double *x)

• void * \( \text{dl} \) \( \text{constructor} \) (Optimizer1 *, Dakota_funcns *, dl_core_run_t *, dl_destructor_t *)
• static RealVector const *continuous_lower_bounds1 (Optimizer1 *o)
• static RealVector const *continuous_upper_bounds1 (Optimizer1 *o)
• static RealVector const *nonlinear_ineq_constraint_lower_bounds1 (Optimizer1 *o)
• static RealVector const *nonlinear_ineq_constraint_upper_bounds1 (Optimizer1 *o)
• static RealVector const *nonlinear_eq_constraint_targets1 (Optimizer1 *o)
• static RealVector const *linear_ineq_constraint_lower_bounds1 (Optimizer1 *o)
• static RealVector const *linear_ineq_constraint_upper_bounds1 (Optimizer1 *o)
• static RealVector const *linear_eq_constraint_targets1 (Optimizer1 *o)
• static RealMatrix const *linear_eq_constraint_coeffs1 (Optimizer1 *o)
• static RealMatrix const *linear_ineq_constraint_coeffs1 (Optimizer1 *o)
• static void ComputeResponses1 (Optimizer1 *o, int mode, int n, double *x)
• static void GetFuncs1 (Optimizer1 *o, int m0, int m1, double *f)
• static void GetGrads1 (Optimizer1 *o, int m0, int m1, int n, int is, int js, double *g)
• static void GetContVars1 (Optimizer1 *o, int n, double *x)
• static void SetBestContVars1 (Optimizer1 *o, int n, double *x)
• static void SetBestDiscVars1 (Optimizer1 *o, int n, int *x)
• static void SetBestRespFns1 (Optimizer1 *o, int n, double *x)
• static double GetReal1 (Optimizer1 *o, const char *name)
• static int GetInt1 (Optimizer1 *o, const char *name)
• static bool GetBool1 (Optimizer1 *o, const char *name)
• DOTOptimizer * new_DOTOptimizer (ProblemDescDB &problem_db)
• DOTOptimizer * new_DOTOptimizer (Model &model)
• void copy_field_data (const RealVector &fn_vals, RealMatrix &fn_grad, const RealSymMatrixArray &fn_hess, size_t offset, size_t num_fns, Response &response)
• void interpolate_simulation_field_data (const Response &sim_resp, const RealMatrix &exp_coords, size_t field_num, short total_asv, size_t interp_resp_offset, Response &interp_resp)
• void linear_interpolate_1d (const RealMatrix &build_pts, const RealVector &build_vals, const RealMatrix &build_grads, const RealSymMatrixArray &build_hessians, const RealMatrix &pred_pts, RealVector &pred_vals, RealMatrix &pred_grads, RealSymMatrixArray &pred_hessians)
  Returns the value of at 1D function f and its gradient and hessians (if available) at the points of vector pred_pts using linear interpolation. The vector build_pts specifies the coordinates of the underlying interval at which the values (build_vals) of the function f are known. The length of output pred_vals is equal to the length of pred_pts. This function assumes the build_pts is in ascending order.
• void symmetric_eigenvalue_decomposition (const RealSymMatrix &matrix, RealVector &eigenvalues, RealMatrix &eigenvectors)
  Computes the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A.
• void compute_column_means (RealMatrix &matrix, RealVector &avg_vals)
  Compute the means of each column of an arbitrary matrix.
• bool is_matrix_symmetric (const RealMatrix &matrix)
  Test if incoming matrix is symmetric.
• template<typename O , typename T >
  int binary_search (T target, Teuchos::SerialDenseVector< O , T > &data)
  find the interval containing a target value. This function assumes the data is in ascending order.
CHAPTER 12. NAMESPACE DOCUMENTATION

- Real getdist (const RealVector &x1, const RealVector &x2)
- Real mindist (const RealVector &x, const RealMatrix &xset, int except)
- Real mindistindx (const RealVector &x, const RealMatrix &xset, const IntArray &indx)
- Real getRmax (const RealMatrix &xset)
- int start_grid_computing (char *analysis_driver_script, char *params_file, char *results_file)
- int stop_grid_computing ()
- int perform_analysis (char *iteration_num)
- template<typename T>
  string asstring (const T &val)
  
  Creates a string from the argument val using an ostringstream.

- PACKBUF (int, MPI_INT) PACKBUF(u_int
- MPI_UNSIGNED PACKBUF (long, MPI_LONG) PACKBUF(u_long
- MPI_UNSIGNED MPI_UNSIGNED_LONG PACKBUF (short, MPI_SHORT) PACKBUF(u_short
- MPI_UNSIGNED MPI_UNSIGNED_LONG 
  MPI_UNSIGNED_SHORT PACKBUF (char, MPI_CHAR) PACKBUF(u_char
- MPI_UNSIGNED MPI_UNSIGNED_LONG 
  MPI_UNSIGNED_SHORT 
  MPI_UNSIGNED_CHAR PACKBUF (double, MPI_DOUBLE) PACKBUF(float
- UNPACKBUF (int, MPI_INT) UNPACKBUF(u_int
- MPI_UNSIGNED UNPACKBUF (long, MPI_LONG) UNPACKBUF(u_long
- MPI_UNSIGNED MPI_UNSIGNED_LONG UNPACKBUF (short, MPI_SHORT) UNPACKBUF(u_short
- MPI_UNSIGNED MPI_UNSIGNED_LONG 
  MPI_UNSIGNED_SHORT UNPACKBUF (char, MPI_CHAR) UNPACKBUF(u_char
- MPI UNSIGNED MPI_UNSIGNED_LONG 
  MPI_UNSIGNED_SHORT 
  MPI_UNSIGNED_CHAR UNPACKBUF (double, MPI DOUBLE) UNPACKBUF(float
- PACKSIZE (int, MPI_INT) PACKSIZE(u_int
- MPI_UNSIGNED PACKSIZE (long, MPI_LONG) PACKSIZE(u_long
- MPI_UNSIGNED MPI_UNSIGNED_LONG PACKSIZE (short, MPI_SHORT) PACKSIZE(u_short
- MPI UNSIGNED MPI_UNSIGNED_LONG 
  MPI_UNSIGNED_SHORT PACKSIZE (char, MPI_CHAR) PACKSIZE(u_char
- MPI_UNSIGNED MPI_UNSIGNED_LONG 
  MPI_UNSIGNED_SHORT 
  MPI_UNSIGNED_CHAR PACKSIZE (double, MPI_DOUBLE) PACKSIZE(float
- MPI_UNSIGNED MPI_UNSIGNED_LONG 
  MPI_UNSIGNED_SHORT 
  MPI_UNSIGNED_CHAR MPI.FLOAT 
  int MPIPackSize (const bool &data, const int num=1)
  
  return packed size of a bool

- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const int &data)
  
  insert an int

- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const u_int &data)
  
  insert a u_int

- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const long &data)
  
  insert a long

- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const u_long &data)
12.1. DAKOTA NAMESPACE REFERENCE

- **MPIPackBuffer & operator<<(MPIPackBuffer &buff, const short &data)**
  
- **MPIPackBuffer & operator<<(MPIPackBuffer &buff, const u_short &data)**
  
- **MPIPackBuffer & operator<<(MPIPackBuffer &buff, const char &data)**
  
- **MPIPackBuffer & operator<<(MPIPackBuffer &buff, const u_char &data)**
  
- **MPIPackBuffer & operator<<(MPIPackBuffer &buff, const double &data)**
  
- **MPIPackBuffer & operator<<(MPIPackBuffer &buff, const float &data)**
  
- **MPIPackBuffer & operator<<(MPIPackBuffer &buff, const bool &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, int &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, u_int &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, long &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, u_long &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, short &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, u_short &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, char &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, u_char &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, double &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, float &data)**
  
- **MPIUnpackBuffer & operator>>(MPIUnpackBuffer &buff, bool &data)**
  
- template&lt;class ContainerT &gt;
  
- void container_read (ContainerT &c, MPIUnpackBuffer &s)
  
    Read a generic container (vector&lt;T&gt;, list&lt;T&gt;) from MPIUnpackBuffer, s.
  
- template&lt;class ContainerT &gt;
  
- void container_write (const ContainerT &c, MPIPackBuffer &s)
  
    Write a generic container to MPIPackBuffer, s.
CHAPTER 12. NAMESPACE DOCUMENTATION

- template<typename Block , typename Allocator >
  MPIPackBuffer & operator<< (MPIPackBuffer &s, const boost::dynamic_bitset< Block, Allocator >&bs)
  
  stream insertion for BitArray

- template<typename Block , typename Allocator >
  MPIUnpackBuffer & operator>>(MPIUnpackBuffer &s, boost::dynamic_bitset< Block, Allocator >&bs)
  
  stream extraction for BitArray

- template<class ContainerT >
  MPIUnpackBuffer & operator>>(MPIUnpackBuffer &s, ContainerT &data)
  
  global MPIUnpackBuffer extraction operator for generic container

- template<class ContainerT >
  MPIPackBuffer & operator<< (MPIPackBuffer &s, const ContainerT &data)
  
  global MPIPackBuffer insertion operator for generic container

- int MPIPackSize (const int &data, const int num=1)
  return packed size of an int

- int MPIPackSize (const u_int &data, const int num=1)
  return packed size of a u_int

- int MPIPackSize (const long &data, const int num=1)
  return packed size of a long

- int MPIPackSize (const u_long &data, const int num=1)
  return packed size of a u_long

- int MPIPackSize (const short &data, const int num=1)
  return packed size of a short

- int MPIPackSize (const u_short &data, const int num=1)
  return packed size of a u_short

- int MPIPackSize (const char &data, const int num=1)
  return packed size of a char

- int MPIPackSize (const u_char &data, const int num=1)
  return packed size of a u_char

- int MPIPackSize (const double &data, const int num=1)
  return packed size of a double

- int MPIPackSize (const float &data, const int num=1)
  return packed size of a float

- int nidr_parse (const char *, FILE *)

- const char ** arg_list_adjust (const char **, void **)

- int not_executable (const char *driver_name, const char *tdir)

- static void scale_chk (StringArray &ST, RealVector &S, const char *what, const char **univ)

- static void BuildLabels (StringArray *sa, size_t nsa, size_t n1, size_t n2, const char *stub)

- static int mixed_check (IntSet *S, int n, IntArray *iv, const char *what)

- static void mixed_check2 (size_t n, IntArray *iv, const char *what)

- static int wronglen (size_t n, RealVector *V, const char *what)

- static int wronglen (size_t n, IntVector *V, const char *what)

- static void Vcopyup (RealVector *V, RealVector *M, size_t i, size_t n)

- static void Set_rv (RealVector *V, double d, size_t n)
12.1. DAKOTA NAMESPACE REFERENCE

- static void Set_iv (IntVector *V, int d, size_t n)
- static void wrong_number (const char *what, const char *kind, size_t nsv, size_t m)
- static void too_small (const char *kind)
- static void not_div (const char *kind, size_t nsv, size_t m)
- static void suppressed (const char *kind, int ndup, int *ip, String *sp, Real *rp)
- static void bad_initial_lvalue (const char *kind, int val)
- static void bad_initial_svalue (const char *kind, String val)
- static void bad_initial_rvalue (const char *kind, Real val)
- static void Vgen_ContinuousDes (DataVariablesRep *dv, size_t offset)
- static void Vgen_DiscreteDesRange (DataVariablesRep *dv, size_t offset)
- static void Vgen_DiscreteStateRange (DataVariablesRep *dv, size_t offset)
- static void Vgen_DiscreteStateRange (DataVariablesRep *dv, size_t offset)
- static void Vchk_NormalUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_LognormalUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_LognormalUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_UniformUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_UniformUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_LoguniformUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_UniformUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_BetaUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_BetaUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_GammaUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_GammaUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_GumbelUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_GumbelUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_FrechetUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_FrechetUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_WeibullUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_WeibullUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_HistogramBinUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)

Check the histogram bin input data, normalize the counts and populate the histogramUncBinPairs map data structure; map keys are guaranteed unique since the abscissas must increase.

- static void Vchk_HistogramBinUnc (DataVariablesRep *dv, size_t offset)

Infer lower/upper bounds for histogram and set initial variable values based on initial_point or moments, snapping to bounds as needed. (Histogram bin doesn’t have lower/upper bounds specification)

- static void Vchk_PoissonUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_PoissonUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_BinomialUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_BinomialUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_NegBinomialUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
- static void Vchk_NegBinomialUnc (DataVariablesRep *dv, size_t offset)
• static void Vchk_GeometricUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_GeometricUnc (DataVariablesRep *dv, size_t offset)
• static void Vchk_HyperGeomUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_HyperGeomUnc (DataVariablesRep *dv, size_t offset)
• static void Vchk_HistogramPtIntUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_HistogramPtIntUnc (DataVariablesRep *dv, size_t offset)
• static void Vchk_HistogramPtStrUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_HistogramPtStrUnc (DataVariablesRep *dv, size_t offset)
• static void Vchk_HistogramPtRealUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_HistogramPtRealUnc (DataVariablesRep *dv, size_t offset)
• static void Vchk_ContinuousIntervalUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_ContinuousIntervalUnc (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteIntervalUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteIntervalUnc (DataVariablesRep *dv, size_t offset)

Check the histogram point integer input data, normalize the counts, and populate DataVariables::histogramUnc-
PointIntPairs; map keys are guaranteed unique since the abscissas must increase.
• static void Vgen_HistogramPtIntUnc (DataVariablesRep *dv, size_t offset)

Use the integer-valued point histogram data to initialize the lower, upper, and initial values of the variables, using
value closest to mean if no initial point.
• static void Vchk_HistogramPtStrUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_HistogramPtStrUnc (DataVariablesRep *dv, size_t offset)

Use the string-valued point histogram data to initialize the lower, upper, and initial values of the variables, using
index closest to mean index if no initial point.
• static void Vchk_HistogramPtRealUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_HistogramPtRealUnc (DataVariablesRep *dv, size_t offset)

Use the real-valued point histogram data to initialize the lower, upper, and initial values of the variables, using
value closest to mean if no initial point.
• static void Vchk_ContinuousIntervalUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_ContinuousIntervalUnc (DataVariablesRep *dv, size_t offset)

Check the continuous interval uncertain input data and populate DataVariables::continuousIntervalUncBasic-
Probs; map keys (real intervals) are checked for uniqueness because we don’t have a theoretically sound way
to combine duplicate intervals.
• static void Vchk_DiscreteIntervalUnc (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteIntervalUnc (DataVariablesRep *dv, size_t offset)

Check the discrete interval uncertain input data and populate DataVariables::discreteIntervalUncBasicProbs; map
keys (integer intervals) are checked for uniqueness because we don’t have a theoretically sound way to combine
duplicate intervals.
• static void Vchk_DSet (size_t num_v, const char *kind, IntArray *input_nds, int &avg_num_ds)
  validate the number of set elements (values) given the number of variables and an optional apportionment with
  elements per variable; return the average number per variable if equally distributed
• static void Vchk_DSet (size_t num_v, const char *kind, IntArray *input_ndsi, IntVector *input_dsi, IntSet-
  Array &dsi_all, IntVector &dsi_init_pt)
  check discrete sets of integers (design and state variables); error if a duplicate value is specified error if not ordered
to prevent user confusion
• static void Vchk_DSet (size_t num_v, const char *kind, IntArray *input_ndsi, IntVector *input_dsi, Real-
  Vector *input_dsip, IntRealMapArray &dsi_vals_probs, IntVector &dsi_init_pt)
  check discrete sets of integers (uncertain variables); error if a duplicate value is specified error if not ordered to
  prevent user confusion
• static void Vchk_DSset (size_t num_v, const char *kind, IntArray *input_ndss, StringArray *input_dss,
  StringSetArray &dss_all, StringArray &dss_init_pt)
• static void Vchk_DSset (size_t num_v, const char *kind, IntArray *input_dss, StringArray *input_dss, RealVector *input_dssp, StringRealMapArray &dss, RealArray &dss_probs, StringArray &dss_init_pt)
• static void Vchk_DSset (size_t num_v, const char *kind, IntArray *input_dsr, RealVector *input_dsrp, RealSetArray &dsr, RealMatrixArray &dda, RealVector &dsr, RealVector &dssr, RealVector &dssrp, RealVector &dsr_all, RealVector &dss_init_pt)
• static void Vchk_Adjacency (size_t num_v, const char *kind, const IntArray &num_e, const IntVector &input_ddsa, RealMatrixArray &dda_all)
• static bool check_LUV_size (size_t num_v, IntVector &L, IntVector &U, IntVector &V, bool aggregate_LUV, size_t offset)
• static bool check_LUV_size (size_t num_v, StringArray &L, StringArray &U, StringArray &V, bool aggregate_LUV, size_t offset)
• static void Vgen_Dset (size_t num_v, IntSetArray &sets, IntVector &L, IntVector &U, IntVector &V, bool aggregate_LUV=false, size_t offset=0)
• static void Vgen_DSet (size_t num_v, StringSetArray &sets, StringArray &L, StringArray &U, StringArray &V, StringArray &U, StringArray &V, bool aggregate_LUV=false, size_t offset=0)

  generate lower, upper, and initial point for string-valued sets
• static void Vchk_DiscreteDesSetInt (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteDesSetInt (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteDesSetInt (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteDesSetInt (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteDesSetStr (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteDesSetStr (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteDesSetReal (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteDesSetReal (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteUncSetInt (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteUncSetInt (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteUncSetInt (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteUncSetInt (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteUncSetReal (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteUncSetReal (DataVariablesRep *dv, size_t offset)
• static void Vchk_DiscreteUncSetReal (DataVariablesRep *dv, size_t offset, Var_Info *vi)
• static void Vgen_DiscreteUncSetReal (DataVariablesRep *dv, size_t offset)
• static const char * Var_Name (StringArray *sa, char *buf, size_t i)
• static void Var_RealBoundIPCheck (DataVariablesRep *dv, Var_rcheck *b)
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For real-valued variables: verify lengths of bounds and initial point, validate bounds and adjust initial point to bounds.

- static void Var_IntBoundIPCheck (DataVariablesRep *dv, Var_check *ib)

For integer-valued variables: verify lengths of bounds and initial point, validate bounds and initial point against bounds.

- static void flatten_rva (RealVectorArray *rva, RealVector **prv)
- static void flatten_iva (IntVectorArray *iva, IntVector **piv)
- static void flatten_rsm (RealSymMatrix *rsm, RealVector **prv)
- static void flatten_rsa (RealSetArray *rsa, RealVector **prv)
- static void flatten_ssa (StringSetArray *ssa, StringArray **psa)
- static void flatten_isa (IntSetArray *isa, IntVector **piv)
- static void flatten_rrma (RealRealMapArray *rrma, RealVector **prv)
- static void flatten_rrma_values (RealRealMapArray *rrma, RealVector **prv)
- static void flatten_irma (IntRealMapArray *irma, IntVector **piv)
- static void flatten_irma_values (IntRealMapArray *irma, RealVector **prv)
- static void flatten_srma (StringRealMapArray *srma, StringArray **psa)
- static void flatten_srma_values (StringRealMapArray *srma, RealVector **prv)
- static void flatten_real_intervals (const RealRealPairRealMapArray &rrprma, RealVector **prv, RealVector **lb, RealVector **ub)
- static void flatten_int_intervals (const IntIntPairRealMapArray &iiprma, RealVector **prv, IntVector **lb, IntVector **ub)

Flatten real-valued interval uncertain variable intervals and probabilities back into separate arrays.

- static void var_iulbl (const char *keyname, Values *val, VarLabel *vl)
- static Iface_mp_Rlit MP3 (failAction, recoveryFnVals, recover)
- static Iface_mp_lit MP3 (failAction, retryLimit, retry)
- static Iface_mp_lit MP2 (failAction, abort)
- static Iface_mp_lit MP2 (failAction, continuation)
- static Iface_mp_type MP2s (analysisScheduling, MASTER_SCHEDULING)
- static Iface_mp_type MP2s (analysisScheduling, PEER_SCHEDULING)
- static Iface_mp_type MP2s (evalScheduling, MASTER_SCHEDULING)
- static Iface_mp_type MP2s (evalScheduling, PEER_DYNAMIC_SCHEDULING)
- static Iface_mp_type MP2s (evalScheduling, PEER_STATIC_SCHEDULING)
- static Iface_mp_type MP2s (asyncLocalEvalScheduling, DYNAMIC_SCHEDULING)
- static Iface_mp_type MP2s (asyncLocalEvalScheduling, STATIC_SCHEDULING)
- static Iface_mp_type MP2s (interfaceSynchronization, ASYNCHRONOUS_INTERFACE)
- static Iface_mp_type MP2s (interfaceSynchronization, SYNCHRONOUS_INTERFACE)
- static Iface_mp_type MP2s (interfaceType, TEST_INTERFACE)
- static Iface_mp_type MP2s (interfaceType, FORK_INTERFACE)
- static Iface_mp_type MP2s (interfaceType, GRID_INTERFACE)
- static Iface_mp_type MP2s (interfaceType, MATLAB_INTERFACE)
- static Iface_mp_type MP2s (interfaceType, PYTHON_INTERFACE)
- static Iface_mp_type MP2s (interfaceType, SCILAB_INTERFACE)
- static Iface_mp_type MP2s (interfaceType, SYSTEM_INTERFACE)
- static Iface_mp_type MP2s (resultsFileFormat, LABELED_RESULTS)
- static String MP (algebraicMappings)
• static String MP_ (idInterface)
• static String MP_ (inputFilter)
• static String MP_ (outputFilter)
• static String MP_ (parametersFile)
• static String MP_ (resultsFile)
• static String MP_ (workDir)
• static String2DArray MP_ (analysisComponents)
• static StringArray MP_ (analysisDrivers)
• static StringArray MP_ (copyFiles)
• static StringArray MP_ (linkFiles)
• static bool MP_ (activeSetVectorFlag)
• static bool MP_ (allowExistingResultsFlag)
• static bool MP_ (apreproFlag)
• static bool MP_ (dirSave)
• static bool MP_ (dirTag)
• static bool MP_ (evalCacheFlag)
• static bool MP_ (fileSaveFlag)
• static bool MP_ (fileTagFlag)
• static bool MP_ (nearbyEvalCacheFlag)
• static bool MP_ (numpyFlag)
• static bool MP_ (restartFileFlag)
• static bool MP_ (templateReplace)
• static bool MP_ (useWorkdir)
• static bool MP_ (verbatimFlag)
• static int MP_ (analysisServers)
• static int MP_ (asynchLocalAnalysisConcurrency)
• static int MP_ (asynchLocalEvalConcurrency)
• static int MP_ (evalServers)
• static int MP_ (procsPerAnalysis)
• static int MP_ (procsPerEval)
• static Real MP_ (nearbyEvalCacheTol)
• static IntVector MP_ (primeBase)
• static IntVector MP_ (refineSamples)
• static IntVector MP_ (sequenceLeap)
• static IntVector MP_ (sequenceStart)
• static IntVector MP_ (stepsPerVariable)
• static Method mp_iliit2 MP3 (replacementType, numberRetained, chc)
• static Method mp_iliit2 MP3 (replacementType, numberRetained, elitist)
• static Method mp_iliit2 MP3 (replacementType, numberRetained, random)
• static Method mp_iliit2z MP3 (crossoverType, numCrossPoints, multi_point_binary)
• static Method mp_iliit2z MP3 (crossoverType, numCrossPoints, multi_point_parameterized_binary)
• static Method mp_iliitz MP3 (crossoverType, numCrossPoints, multi_point_real)
• static Method mp_lit MP2 (batchSelectionType, naive)
• static Method mp_lit MP2 (batchSelectionType, distance_penalty)
• static Method mp_lit MP2 (batchSelectionType, topology)
• static Method mp_lit MP2 (batchSelectionType, constant liar)
- static Method _mp_lit MP2 (boxDivision, all_dimensions)
- static Method _mp_lit MP2 (boxDivision, major_dimension)
- static Method _mp_lit MP2 (convergenceType, average_fitness_tracker)
- static Method _mp_lit MP2 (convergenceType, best_fitness_tracker)
- static Method _mp_lit MP2 (convergenceType, metric_tracker)
- static Method _mp_lit MP2 (crossoverType, blend)
- static Method _mp_lit MP2 (crossoverType, two_point)
- static Method _mp_lit MP2 (crossoverType, uniform)
- static Method _mp_lit MP2 (dataDistCovInputType, diagonal)
- static Method _mp_lit MP2 (dataDistCovInputType, matrix)
- static Method _mp_lit MP2 (discrepancyType, global_kriging)
- static Method _mp_lit MP2 (discrepancyType, global_polynomial)
- static Method _mp_lit MP2 (evalSynchronize, blocking)
- static Method _mp_lit MP2 (evalSynchronize, nonblocking)
- static Method _mp_lit MP2 (expansionSampleType, incremental_lhs)
- static Method _mp_lit MP2 (exploratoryMoves, adaptive)
- static Method _mp_lit MP2 (exploratoryMoves, multi_step)
- static Method _mp_lit MP2 (exploratoryMoves, simple)
- static Method _mp_lit MP2 (fitnessType, domination_count)
- static Method _mp_lit MP2 (fitnessType, layer_rank)
- static Method _mp_lit MP2 (fitnessType, linear_rank)
- static Method _mp_lit MP2 (fitnessType, merit_function)
- static Method _mp_lit MP2 (fitnessType, proportional)
- static Method _mp_lit MP2 (fitnessMetricType, predicted_variance)
- static Method _mp_lit MP2 (fitnessMetricType, distance)
- static Method _mp_lit MP2 (fitnessMetricType, gradient)
- static Method _mp_lit MP2 (initializationType, random)
- static Method _mp_lit MP2 (initializationType, unique_random)
- static Method _mp_lit MP2 (lipschitzType, global)
- static Method _mp_lit MP2 (lipschitzType, local)
- static Method _mp_lit MP2 (meritFunction, merit_max)
- static Method _mp_lit MP2 (meritFunction, merit_max_smooth)
- static Method _mp_lit MP2 (meritFunction, merit1)
- static Method _mp_lit MP2 (meritFunction, merit1_smooth)
- static Method _mp_lit MP2 (meritFunction, merit2)
- static Method _mp_lit MP2 (meritFunction, merit2_smooth)
- static Method _mp_lit MP2 (meritFunction, merit2_squared)
- static Method _mp_lit MP2 (mcmcType, adaptive_metropolis)
- static Method _mp_lit MP2 (mcmcType, delayed_rejection)
- static Method _mp_lit MP2 (mcmcType, dram)
- static Method _mp_lit MP2 (mcmcType, metropolis_hastings)
- static Method _mp_lit MP2 (mcmcType, multilevel)
- static Method _mp_lit MP2 (mutationType, bit_random)
- static Method _mp_lit MP2 (mutationType, offset_cauchy)
- static Method _mp_lit MP2 (mutationType, offset_normal)
- static Method _mp_lit MP2 (mutationType, offset_uniform)
• static Method\textunderscore mp\textunderscore lit MP2 (mutationType, replace\_uniform)
• static Method\textunderscore mp\textunderscore lit MP2 (patternBasis, coordinate)
• static Method\textunderscore mp\textunderscore lit MP2 (patternBasis, simplex)
• static Method\textunderscore mp\textunderscore lit MP2 (pointReuse, all)
• static Method\textunderscore mp\textunderscore lit MP2 (proposalCovInputType, diagonal)
• static Method\textunderscore mp\textunderscore lit MP2 (proposalCovInputType, matrix)
• static Method\textunderscore mp\textunderscore lit MP2 (proposalCovType, derivatives)
• static Method\textunderscore mp\textunderscore lit MP2 (proposalCovType, prior)
• static Method\textunderscore mp\textunderscore lit MP2 (proposalCovType, user)
• static Method\textunderscore mp\textunderscore lit MP2 (reliabilityIntegration, first\_order)
• static Method\textunderscore mp\textunderscore lit MP2 (reliabilityIntegration, second\_order)
• static Method\textunderscore mp\textunderscore lit MP2 (replacementType, elitist)
• static Method\textunderscore mp\textunderscore lit MP2 (replacementType, favor\_feasible)
• static Method\textunderscore mp\textunderscore lit MP2 (replacementType, roulette\_wheel)
• static Method\textunderscore mp\textunderscore lit MP2 (replacementType, unique\_roulette\_wheel)
• static Method\textunderscore mp\textunderscore lit MP2 (rngName, mt19937)
• static Method\textunderscore mp\textunderscore lit MP2 (rngName, rnum2)
• static Method\textunderscore mp\textunderscore lit MP2 (searchMethod, gradient\_based\_line\_search)
• static Method\textunderscore mp\textunderscore lit MP2 (searchMethod, tr\_pds)
• static Method\textunderscore mp\textunderscore lit MP2 (searchMethod, trust\_region)
• static Method\textunderscore mp\textunderscore lit MP2 (searchMethod, value\_based\_line\_search)
• static Method\textunderscore mp\textunderscore lit MP2 (trialType, grid)
• static Method\textunderscore mp\textunderscore lit MP2 (trialType, halton)
• static Method\textunderscore mp\textunderscore lit MP2 (trialType, random)
• static Method\textunderscore mp\textunderscore lit MP2 (useSurrogate, inform\_search)
• static Method\textunderscore mp\textunderscore lit MP2 (useSurrogate, optimize)
• static Method\textunderscore mp\textunderscore ltc MP3 (crossoverType, crossoverRate, shuffle\_random)
• static Method\textunderscore mp\textunderscore ltc MP3 (crossoverType, crossoverRate, null\_crossover)
• static Method\textunderscore mp\textunderscore ltc MP3 (mutationType, mutationRate, null\_mutation)
• static Method\textunderscore mp\textunderscore ltc MP3 (mutationType, mutationRate, offset\_cauchy)
• static Method\textunderscore mp\textunderscore ltc MP3 (mutationType, mutationRate, offset\_normal)
• static Method\textunderscore mp\textunderscore ltc MP3 (mutationType, mutationRate, offset\_uniform)
• static Method\textunderscore mp\textunderscore ltc MP3 (replacementType, fitnessLimit, below\_limit)
• static Method\textunderscore mp\textunderscore litrv MP3 (nichingType, nicheVector, distance)
• static Method\textunderscore mp\textunderscore litrv MP3 (nichingType, nicheVector, max\_designs)
• static Method\textunderscore mp\textunderscore litrv MP3 (nichingType, nicheVector, radial)
• static Method\textunderscore mp\textunderscore litrv MP3 (postProcessorType, distanceVector, distance\_postprocessor)
• static Method\textunderscore mp\textunderscore slit2 MP3 (initializationType, flatFile, flat\_file)
• static Method\textunderscore mp\textunderscore utype\_lit MP3s (methodName, dlDetails, DL\_SOLVER)
• static Method\textunderscore mp\textunderscore ord MP2s (approxCorrectionOrder, 0)
• static Method\textunderscore mp\textunderscore ord MP2s (approxCorrectionOrder, 1)
• static Method\textunderscore mp\textunderscore ord MP2s (approxCorrectionOrder, 2)
• static Real MP\textunderscore absConvTol
• static Real MP\textunderscore centeringParam
• static Real MP\textunderscore collocationRatio
• static Real MP\textunderscore collocRatioTermsOrder
- static Real MP_ (constraintPenalty)
- static Real MP_ (constrPenalty)
- static Real MP_ (constraintTolerance)
- static Real MP_ (contractFactor)
- static Real MP_ (contractStepLength)
- static Real MP_ (convergenceTolerance)
- static Real MP_ (crossoverRate)
- static Real MP_ (falseConvTol)
- static Real MP_ (functionPrecision)
- static Real MP_ (globalBalanceParam)
- static Real MP_ (gradientTolerance)
- static Real MP_ (hybridLSProb)
- static Real MP_ (grThreshold)
- static Real MP_ (initDelta)
- static Real MP_ (initMeshSize)
- static Real MP_ (initStepLength)
- static Real MP_ (initTRRadius)
- static Real MP_ (lineSearchTolerance)
- static Real MP_ (localBalanceParam)
- static Real MP_ (maxBoxSize)
- static Real MP_ (maxStep)
- static Real MP_ (minBoxSize)
- static Real MP_ (minMeshSize)
- static Real MP_ (mutationRate)
- static Real MP_ (mutationScale)
- static Real MP_ (percentVarianceExplained)
- static Real MP_ (refinementRate)
- static Real MP_ (regressionL2Penalty)
- static Real MP_ (shrinkagePercent)
- static Real MP_ (singConvTol)
- static Real MP_ (singRadius)
- static Real MP_ (smoothFactor)
- static Real MP_ (solnTarget)
- static Real MP_ (stepLenToBoundary)
- static Real MP_ (threshDelta)
- static Real MP_ (threshStepLength)
- static Real MP_ (trustRegionContract)
- static Real MP_ (trustRegionContractTrigger)
- static Real MP_ (trustRegionExpand)
- static Real MP_ (trustRegionExpandTrigger)
- static Real MP_ (trustRegionMinSize)
- static Real MP_ (vbdDropTolerance)
- static Real MP_ (volBoxSize)
- static Real MP_ (vns)
- static Real MP_ (wilksConfidenceLevel)
- static Real MP_ (xConvTol)
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- static RealVector MP_ (anisoDimPref)
- static RealVector MP_ (concurrentParameterSets)
- static RealVector MP_ (dataDistCovariance)
- static RealVector MP_ (dataDistMeans)
- static RealVector MP_ (finalPoint)
- static RealVector MP_ (hyperPriorAlphas)
- static RealVector MP_ (hyperPriorBetas)
- static RealVector MP_ (listOfPoints)
- static RealVector MP_ (predictionConfigList)
- static RealVector MP_ (proposalCovData)
- static RealVector MP_ (regressionNoiseTol)
- static RealVector MP_ (stepVector)
- static RealVector MP_ (trustRegionInitSize)
- static RealVectorArray MP_ (genReliabilityLevels)
- static RealVectorArray MP_ (probabilityLevels)
- static RealVectorArray MP_ (reliabilityLevels)
- static RealVectorArray MP_ (responseLevels)
- static unsigned short MP_ (adaptedBasisAdvancements)
- static unsigned short MP_ (cubIntOrder)
- static unsigned short MP_ (softConvLimit)
- static unsigned short MP_ (vbdOrder)
- static unsigned short MP_ (wilksOrder)
- static SizetArray MP_ (collocationPoints)
- static SizetArray MP_ (expansionSamples)
- static SizetArray MP_ (pilotSamples)
- static UShortArray MP_ (expansionOrder)
- static UShortArray MP_ (quadratureOrder)
- static UShortArray MP_ (sparseGridLevel)
- static UShortArray MP_ (tensorGridOrder)
- static UShortArray MP_ (varPartitions)
- static String MP_ (betaSolverName)
- static String MP_ (dataDistFile)
- static String MP_ (displayFormat)
- static String MP_ (exportApproxPtsFile)
- static String MP_ (exportCorrModelFile)
- static String MP_ (exportCorrVarFile)
- static String MP_ (exportDiscrepFile)
- static String MP_ (exportExpansionFile)
- static String MP_ (exportMCMCPtsFile)
- static String MP_ (historyFile)
- static String MP_ (hybridGlobalMethodName)
- static String MP_ (hybridGlobalMethodPointer)
- static String MP_ (hybridGlobalModelPointer)
- static String MP_ (hybridLocalMethodName)
- static String MP_ (hybridLocalMethodPointer)
- static String MP_ (hybridLocalModelPointer)
• static String \texttt{MP}_c (idMethod)
• static String \texttt{MP}_c (importApproxPtsFile)
• static String \texttt{MP}_c (importBuildPtsFile)
• static String \texttt{MP}_c (importCandPtsFile)
• static String \texttt{MP}_c (importExpansionFile)
• static String \texttt{MP}_c (importPredConfigs)
• static String \texttt{MP}_c (logFile)
• static String \texttt{MP}_c (lowFidModelPointer)
• static String \texttt{MP}_c (modelPointer)
• static String \texttt{MP}_c (posteriorDensityExportFilename)
• static String \texttt{MP}_c (posteriorSamplesExportFilename)
• static String \texttt{MP}_c (posteriorSamplesImportFilename)
• static String \texttt{MP}_c (proposalCovFile)
• static String \texttt{MP}_c (pstudyFilename)
• static String \texttt{MP}_c (quesoOptionsFilename)
• static String \texttt{MP}_c (subMethodName)
• static String \texttt{MP}_c (subMethodPointer)
• static String \texttt{MP}_c (subModelPointer)
• static StringArray \texttt{MP}_c (hybridMethodNames)
• static StringArray \texttt{MP}_c (hybridMethodPointers)
• static StringArray \texttt{MP}_c (hybridModelPointers)
• static StringArray \texttt{MP}_c (miscOptions)
• static bool \texttt{MP}_c (adaptExpDesign)
• static bool \texttt{MP}_c (adaptPosteriorRefine)
• static bool \texttt{MP}_c (backfillFlag)
• static bool \texttt{MP}_c (calModelDiscrepancy)
• static bool \texttt{MP}_c (constantPenalty)
• static bool \texttt{MP}_c (crossValidation)
• static bool \texttt{MP}_c (crossValidNoiseOnly)
• static bool \texttt{MP}_c (dOptimal)
• static bool \texttt{MP}_c (evaluatePosteriorDensity)
• static bool \texttt{MP}_c (expansionFlag)
• static bool \texttt{MP}_c (exportSampleSeqFlag)
• static bool \texttt{MP}_c (fixedSeedFlag)
• static bool \texttt{MP}_c (fixedSequenceFlag)
• static bool \texttt{MP}_c (generatePosteriorSamples)
• static bool \texttt{MP}_c (gpmsaNormalize)
• static bool \texttt{MP}_c (importApproxActive)
• static bool \texttt{MP}_c (importBuildActive)
• static bool \texttt{MP}_c (latinizeFlag)
• static bool \texttt{MP}_c (logitTransform)
• static bool \texttt{MP}_c (mainEffectsFlag)
• static bool \texttt{MP}_c (methodScaling)
• static bool \texttt{MP}_c (methodUseDerivsFlag)
• static bool \texttt{MP}_c (mutationAdaptive)
• static bool \texttt{MP}_c (normalizedCoeffs)
• static bool MP_x (pcaFlag)
• static bool MP_x (posteriorStatsKL)
• static bool MP_x (posteriorStatsMutual)
• static bool MP_x (printPopFlag)
• static bool MP_x (pstudyFileActive)
• static bool MP_x (randomizeOrderFlag)
• static bool MP_x (regressDiag)
• static bool MP_x (showAllEval)
• static bool MP_x (showMiscOptions)
• static bool MP_x (speculativeFlag)
• static bool MP_x (standardizedSpace)
• static bool MP_x (tensorGridFlag)
• static bool MP_x (surrBasedGlobalReplacePts)
• static bool MP_x (surrBasedLocalLayerBypass)
• static bool MP_x (vbdFlag)
• static bool MP_x (volQualityFlag)
• static bool MP_x (wilksFlag)
• static short MP_x (expansionType)
• static short MP_x (nestingOverride)
• static short MP_x (refinementType)
• static short MP_x (wilksSidedInterval)
• static int MP_x (buildSamples)
• static int MP_x (burnInSamples)
• static int MP_x (chainSamples)
• static int MP_x (concurrentRandomJobs)
• static int MP_x (contractAfterFail)
• static int MP_x (covarianceType)
• static int MP_x (crossoverChainPairs)
• static int MP_x (emulatorOrder)
• static int MP_x (expandAfterSuccess)
• static int MP_x (iteratorServers)
• static int MP_x (jumpStep)
• static int MP_x (maxFunctionEvaluations)
• static int MP_x (maxHifiEvals)
• static int MP_x (maxIterations)
• static int MP_x (maxRefineIterations)
• static int MP_x (maxSolverIterations)
• static int MP_x (mutationRange)
• static int MP_x (neighborOrder)
• static int MP_x (newSolnsGenerated)
• static int MP_x (numChains)
• static int MP_x (numCR)
• static int MP_x (numSamples)
• static int MP_x (numSteps)
• static int MP_x (numSymbols)
• static int MP_x (numTrials)
• static int MP_ (populationSize)
• static int MP_ (procsPerIterator)
• static int MP_ (proposalCovUpdates)
• static int MP_ (randomSeed)
• static int MP_ (samplesOnEmulator)
• static int MP_ (searchSchemeSize)
• static int MP_ (subSamplingPeriod)
• static int MP_ (totalPatternSize)
• static int MP_ (verifyLevel)
• static size_t MP_ (numCandidateDesigns)
• static size_t MP_ (numCandidates)
• static size_t MP_ (numDesigns)
• static size_t MP_ (numFinalSolutions)
• static size_t MP_ (numGenerations)
• static size_t MP_ (numOffspring)
• static size_t MP_ (numParents)
• static size_t MP_ (numPredConfigs)
• static Method mp_type MP2s (covarianceControl, DIAGONAL_COVARIANCE)
• static Method mp_type MP2s (covarianceControl, FULL_COVARIANCE)
• static Method mp_type MP2s (distributionType, COMPLEMENTARY)
• static Method mp_type MP2s (distributionType, CUMULATIVE)
• static Method mp_type MP2s (emulatorType, GP_EMULATOR)
• static Method mp_type MP2s (emulatorType, KRIGING_EMULATOR)
• static Method mp_type MP2s (emulatorType, PCE_EMULATOR)
• static Method mp_type MP2s (emulatorType, SC_EMULATOR)
• static Method mp_type MP2s (emulatorType, VPS_EMULATOR)
• static Method mp_type MP2p (expansionBasisType, ADAPTED_BASIS_EXPANDING_FRONT)
• static Method mp_type MP2p (expansionBasisType, ADAPTED_BASIS_GENERALIZED)
• static Method mp_type MP2p (expansionBasisType, HIERARCHICAL_INTERPOLANT)
• static Method mp_type MP2p (expansionBasisType, NODAL_INTERPOLANT)
• static Method mp_type MP2p (expansionBasisType, TENSOR_PRODUCT_BASIS)
• static Method mp_type MP2p (expansionBasisType, TOTAL_ORDER_BASIS)
• static Method mp_type MP2s (expansionType, ASKEY_U)
• static Method mp_type MP2s (expansionType, STD_NORMAL_U)
• static Method mp_type MP2s (finalMomentsType, CENTRAL_MOMENTS)
• static Method mp_type MP2s (finalMomentsType, NO_MOMENTS)
• static Method mp_type MP2s (finalMomentsType, STANDARD_MOMENTS)
• static Method mp_type MP2p (growthOverride, RESTRICTED)
• static Method mp_type MP2p (growthOverride, UNRESTRICTED)
• static Method mp_type MP2s (iteratorScheduling, MASTER_SCHEDULING)
• static Method mp_type MP2s (iteratorScheduling, PEER_SCHEDULING)
• static Method mp_type MP2s (lsRegressionType, EQ_CON_LS)
• static Method mp_type MP2s (lsRegressionType, SVD_LS)
• static Method mp_type MP2o (meritFn, ArgaezTapia)
• static Method mp_type MP2o (meritFn, NormFmu)
• static Method mp_type MP2o (meritFn, VanShanno)
• static Method mp_type MP2s (methodOutput, DEBUG_OUTPUT)
• static Method mp_type MP2s (methodOutput, NORMAL_OUTPUT)
• static Method mp_type MP2s (methodOutput, QUIET_OUTPUT)
• static Method mp_type MP2s (methodOutput, SILENT_OUTPUT)
• static Method mp_type MP2s (methodOutput, VERBOSE_OUTPUT)
• static Method mp_type MP2p (nestingOverride, NESTED)
• static Method mp_type MP2p (nestingOverride, NON_NESTED)
• static Method mp_type MP2p (refinementControl, DIMENSION_ADAPTIVE_CONTROL_GENERALIZED)
• static Method mp_type MP2p (refinementControl, DIMENSION_ADAPTIVE_CONTROL_DECAY)
• static Method mp_type MP2p (refinementControl, LOCAL_ADAPTIVE_CONTROL)
• static Method mp_type MP2p (refinementControl, UNIFORM_CONTROL)
• static Method mp_type MP2p (refinementType, P_REFINEMENT)
• static Method mp_type MP2p (refinementType, H_REFINEMENT)
• static Method mp_type MP2p (regressionType, BASIS_PURSUIT)
• static Method mp_type MP2p (regressionType, BASIS_PURSUIT_DENOISING)
• static Method mp_type MP2p (regressionType, DEFAULT_LEAST_SQ_REGRESSION)
• static Method mp_type MP2p (regressionType, LASSO_REGRESSION)
• static Method mp_type MP2p (regressionType, LEAST_ANGLE_REGRESSION)
• static Method mp_type MP2p (regressionType, ORTHOG_LEAST_INTERPOLATION)
• static Method mp_type MP2p (regressionType, ORTHOG_MATCH_PURSUIT)
• static Method mp_type MP2s (responseLevelTarget, GEN_RELIABILITIES)
• static Method mp_type MP2s (responseLevelTarget, PROBABILITIES)
• static Method mp_type MP2s (responseLevelTarget, RELIABILITIES)
• static Method mp_type MP2s (responseLevelTargetReduce, SYSTEM_PARALLEL)
• static Method mp_type MP2s (responseLevelTargetReduce, SYSTEM_SERIES)
• static Method mp_type MP2s (surrBasedLocalAcceptLogic, FILTER)
• static Method mp_type MP2s (surrBasedLocalAcceptLogic, TR_RATIO)
• static Method mp_type MP2s (surrBasedLocalConstrRelax, HOMOTOPY)
• static Method mp_type MP2p (surrBasedLocalMeritFn, ADAPTIVE_PENALTY_MERIT)
• static Method mp_type MP2p (surrBasedLocalMeritFn, AUGMENTED_LAGRANGIAN_MERIT)
• static Method mp_type MP2s (surrBasedLocalSubProbCon, LINEARIZED_CONSTRAINTS)
• static Method mp_type MP2s (surrBasedLocalSubProbCon, NO_CONSTRAINTS)
• static Method mp_type MP2s (surrBasedLocalSubProbObj, AUGMENTED_LAGRANGIAN_OBJECTIVE)
• static Method mp_type MP2s (surrBasedLocalSubProbObj, LAGRANGIAN_OBJECTIVE)
• static Method mp_type MP2s (surrBasedLocalSubProbObj, ORIGINAL_PRIMARY)
• static Method mp_type MP2s (surrBasedLocalSubProbObj, SINGLE_OBJECTIVE)
• static Method mp_type MP2s (wilksSidedInterval, ONE_SIDED_LOWER)
• static Method mp_type MP2s (wilksSidedInterval, ONE_SIDED_UPPER)
• static Method mp_type MP2s (wilksSidedInterval, TWO_SIDED)
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static Method:_mp_ubyte MP2s (calibrateErrorMode, CALIBRATE_PER_RESP)
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• static Method_mp_utype MP2s (methodName, COLINY_COBYLA)
• static Method_mp_utype MP2s (methodName, COLINY_DIRECT)
• static Method_mp_utype MP2s (methodName, COLINY_EA)
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• static Method_mp_utype MP2s (methodName, FSU_HALTON)
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• static Method_mp_utype MP2s (methodName, NLSSOL_SQP)
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• static Method_mp_utype MP2s (subMethod, SUBMETHOD_CONVERGE_QOI)
• static Method_mp_utype MP2s (subMethod, SUBMETHOD_ESTIMATE_ORDER)
• static IntSet MP_ (surrogateFnIndices)
• static Model_mp_lit MP2 (approxPointReuse, all)
• static Model_mp_lit MP2 (approxPointReuse, none)
• static Model_mp_lit MP2 (approxPointReuse, region)
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• static Model_mp_lit MP2 (marsInterpolation, cubic)
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• static Model_mp_lit MP2 (modelType, adapted_basis)
• static Model_mp_lit MP2 (modelType, nested)
• static Model_mp_lit MP2 (modelType, random_field)
• static Model_mp_lit MP2 (modelType, simulation)
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• static Model_mp_lit MP2 (surrogateType, global_neural_network)
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• static Model_mp_lit MP2 (surrogateType, global_voronoi_surrogate)
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• static Model\_mp\_lit MP2 (trendOrder, quadratic)
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• static Model\_mp\_ord MP2s (polynomialOrder, 2)
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• static Model\_mp\_type MP2s (pointsManagement, RECOMMENDED\_POINTS)
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• static Model\_mp\_type MP2s (subMethodScheduling, PEER\_SCHEDULING)
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• static Real MP\_ (truncationTolerance)
• static Real MP\_ (relTolerance)
• static Real MP\_ (decreaseTolerance)
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• static RealVector MP\_ (secondaryRespCoeffs)
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• static StringArray M\textsubscript{P} (secondaryVarMaps)
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• static bool M\textsubscript{P} (decompDiscontDetect)
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• static int \texttt{MP\_}(subMethodServers)
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• static int \texttt{MP\_}(subspaceCVMaxRank)
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• static \texttt{IntSet}\texttt{MP\_}(idAnalyticHessians)
• static \texttt{IntSet}\texttt{MP\_}(idNumericalGrads)
• static \texttt{IntSet}\texttt{MP\_}(idNumericalHessians)
• static \texttt{IntSet}\texttt{MP\_}(idQuasiHessians)
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• static \texttt{IntVector}\texttt{MP\_}(numCoordsPerField)
• static \texttt{RealVector}\texttt{MP\_}(expConfigVars)
• static \texttt{RealVector}\texttt{MP\_}(expObservations)
• static \texttt{RealVector}\texttt{MP\_}(primaryRespFnWeights)
• static \texttt{RealVector}\texttt{MP\_}(nonlinearEqTargets)
• static \texttt{RealVector}\texttt{MP\_}(nonlinearIneqLowerBnds)
• static \texttt{RealVector}\texttt{MP\_}(nonlinearIneqUpperBnds)
• static \texttt{RealVector}\texttt{MP\_}(fdGradStepSize)
• static \texttt{RealVector}\texttt{MP\_}(fdHessStepSize)
• static \texttt{RealVector}\texttt{MP\_}(primaryRespFnScales)
• static \texttt{RealVector}\texttt{MP\_}(nonlinearEqScales)
• static \texttt{RealVector}\texttt{MP\_}(nonlinearIneqScales)
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• static \texttt{Resp\_mp\_lit} \texttt{MP2}(gradientType, mixed)
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• static \texttt{Resp\_mp\_lit} \texttt{MP2}(gradientType, numerical)
• static \texttt{Resp\_mp\_lit} \texttt{MP2}(hessianType, analytic)
• static \texttt{Resp\_mp\_lit} \texttt{MP2}(hessianType, mixed)
• static \texttt{Resp\_mp\_lit} \texttt{MP2}(hessianType, none)
• static \texttt{Resp\_mp\_lit} \texttt{MP2}(hessianType, numerical)
• static \texttt{Resp\_mp\_lit} \texttt{MP2}(hessianType, quasi)
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• static \texttt{Resp\_mp\_lit} \texttt{MP2}(intervalType, forward)
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• static \texttt{Resp\_mp\_lit} \texttt{MP2}(methodSource, vendor)
• static \texttt{Resp\_mp\_lit} \texttt{MP2}(fdGradStepType, absolute)
• static Resp_mp_lit MP2 (fdGradStepType, bounds)
• static Resp_mp_lit MP2 (fdGradStepType, relative)
• static Resp_mp_lit MP2 (fdHessStepType, absolute)
• static Resp_mp_lit MP2 (fdHessStepType, bounds)
• static Resp_mp_lit MP2 (fdHessStepType, relative)
• static Resp_mp_lit MP2 (quasiHessianType, bfgs)
• static Resp_mp_lit MP2 (quasiHessianType, damped_bfgs)
• static Resp_mp_lit MP2 (quasiHessianType, sr1)
• static String MP_ (scalarDataFileName)
• static String MP_ (idResponses)
• static StringArray MP_ (nonlinearEqScaleTypes)
• static StringArray MP_ (nonlinearIneqScaleTypes)
• static StringArray MP_ (primaryRespFnScaleTypes)
• static StringArray MP_ (primaryRespFnSense)
• static StringArray MP_ (responseLabels)
• static bool MP_ (calibrationDataFlag)
• static bool MP_ (centralHess)
• static bool MP_ (interpolateFlag)
• static bool MP_ (ignoreBounds)
• static bool MP_ (readFieldCoords)
• static size_t MP_ (numExpConfigVars)
• static size_t MP_ (numExperiments)
• static size_t MP_ (numFieldLeastSqTerms)
• static size_t MP_ (numFieldObjectiveFunctions)
• static size_t MP_ (numFieldResponseFunctions)
• static size_t MP_ (numLeastSqTerms)
• static size_t MP_ (numNonlinearEqConstraints)
• static size_t MP_ (numNonlinearIneqConstraints)
• static size_t MP_ (numScalarLeastSqTerms)
• static size_t MP_ (numScalarObjectiveFunctions)
• static size_t MP_ (numScalarResponseFunctions)
• static Resp_mp_utype MP2s (scalarDataFormat, TABULAR_NONE)
• static Resp_mp_utype MP2s (scalarDataFormat, TABULAR_HEADER)
• static Resp_mp_utype MP2s (scalarDataFormat, TABULAR_EVAL_ID)
• static Resp_mp_utype MP2s (scalarDataFormat, TABULAR_EXPER_ANNOT)
• static Env_mp_utype MP2s (postRunInputFormat, TABULAR_NONE)
• static Env_mp_utype MP2s (postRunInputFormat, TABULAR_HEADER)
• static Env_mp_utype MP2s (postRunInputFormat, TABULAR_EVAL_ID)
• static Env_mp_utype MP2s (postRunInputFormat, TABULAR_IFACE_ID)
• static Env_mp_utype MP2s (preRunOutputFormat, TABULAR_NONE)
• static Env_mp_utype MP2s (preRunOutputFormat, TABULAR_HEADER)
• static Env_mp_utype MP2s (preRunOutputFormat, TABULAR_EVAL_ID)
- static Env_mp_utype MP2s (preRunOutputFormat, TABULAR_IFACE_ID)
- static Env_mp_utype MP2s (preRunOutputFormat, TABULAR_ANNOTATED)
- static Env_mp_utype MP2s (tabularFormat, TABULAR_NONE)
- static Env_mp_utype MP2s (tabularFormat, TABULAR_HEADER)
- static Env_mp_utype MP2s (tabularFormat, TABULAR_EVAL_ID)
- static Env_mp_utype MP2s (tabularFormat, TABULAR_IFACE_ID)
- static Env_mp_utype MP2s (tabularFormat, TABULAR_ANNOTATED)
- static String MP_ (errorFile)
- static String MP_ (outputFile)
- static String MP_ (postRunInput)
- static String MP_ (postRunOutput)
- static String MP_ (preRunInput)
- static String MP_ (preRunOutput)
- static String MP_ (readRestart)
- static String MP_ (resultsOutputFile)
- static String MP_ (runInput)
- static String MP_ (runOutput)
- static String MP_ (tabularDataFile)
- static String MP_ (topMethodPointer)
- static String MP_ (writeRestart)
- static bool MP_ (checkFlag)
- static bool MP_ (graphicsFlag)
- static bool MP_ (postRunFlag)
- static bool MP_ (preRunFlag)
- static bool MP_ (resultsOutputFlag)
- static bool MP_ (runFlag)
- static bool MP_ (tabularDataFlag)
- static int MP_ (outputPrecision)
- static int MP_ (stopRestart)
- static size_t MP_ (numBetaUncVars)
- static size_t MP_ (numBinomialUncVars)
- static size_t MP_ (numContinuousDesVars)
- static size_t MP_ (numContinuousIntervalUncVars)
- static size_t MP_ (numContinuousStateVars)
- static size_t MP_ (numDiscreteDesRangeVars)
- static size_t MP_ (numDiscreteDesSetIntVars)
- static size_t MP_ (numDiscreteDesSetStrVars)
- static size_t MP_ (numDiscreteDesSetRealVars)
- static size_t MP_ (numDiscreteIntervalUncVars)
- static size_t MP_ (numDiscreteStateRangeVars)
- static size_t MP_ (numDiscreteStateSetIntVars)
- static size_t MP_ (numDiscreteStateSetStrVars)
- static size_t MP_ (numDiscreteUncSetIntVars)
- static size_t MP_ (numDiscreteUncSetStrVars)
- static size_t MP_ (numDiscreteUncSetRealVars)
12.1. **DAKOTA NAMESPACE REFERENCE**

- static `size_t` MP (numExponentialUncVars)
- static `size_t` MP (numFrechetUncVars)
- static `size_t` MP (numGammaUncVars)
- static `size_t` MP (numGeometricUncVars)
- static `size_t` MP (numGumbelUncVars)
- static `size_t` MP (numHistogramBinUncVars)
- static `size_t` MP (numHistogramPtIntUncVars)
- static `size_t` MP (numHistogramPtStrUncVars)
- static `size_t` MP (numHistogramPtRealUncVars)
- static `size_t` MP (numHyperGeomUncVars)
- static `size_t` MP (numLognormalUncVars)
- static `size_t` MP (numLoguniformUncVars)
- static `size_t` MP (numNegBinomialUncVars)
- static `size_t` MP (numNormalUncVars)
- static `size_t` MP (numPoissonUncVars)
- static `size_t` MP (numTriangularUncVars)
- static `size_t` MP (numUniformUncVars)
- static `size_t` MP (numWeibullUncVars)
- static `IntVector` VP (dssi)
- static `IntVector` VP (DIlb)
- static `IntVector` MP (discreteDesignRangeLowerBnds)
- static `IntVector` MP (discreteDesignRangeUpperBnds)
- static `IntVector` MP (discreteDesignRangeVars)
- static `IntVector` MP (discreteDesignSetIntVars)
- static `IntVector` MP (discreteIntervalUncVars)
- static `IntVector` MP (discreteStateRangeLowerBnds)
- static `IntVector` MP (discreteStateRangeUpperBnds)
- static `IntVector` MP (discreteStateRangeVars)
- static `IntVector` MP (discreteStateSetIntVars)
- static `IntVector` MP (discreteUncSetIntVars)
- static `IntVector` VP (DItub)
- static `IntVector` MP (histogramPointIntUncVars)
- static `IntVector` VP (hpia)
- static `IntVector` VP (dssi)
- static `IntVector` VP (ddsia)
- static `IntVector` VP (ddssa)
- static `IntVector` VP (ddsra)
- static `IntVector` VP (ddss)
- static `IntArray` VP (ndds)
- static `IntArray` VP (nddss)
- static `IntArray` VP (nddsr)
- static `IntArray` VP (nddsis)
- static `IntArray` VP (nddsr)
- static `IntArray` VP (nduss)
- static IntArray VP_ (ndusr)
- static IntArray VP_ (nhbp)
- static IntArray VP_ (nhpip)
- static IntArray VP_ (nhpsp)
- static IntArray VP_ (nhprp)
- static IntArray VP_ (nCI)
- static IntArray VP_ (nDI)
- static RealVector MP_ (betaUncLowerBnds)
- static RealVector MP_ (betaUncUpperBnds)
- static RealVector MP_ (betaUncVars)
- static RealVector MP_ (binomialUncProbPerTrial)
- static RealVector MP_ (continuousDesignLowerBnds)
- static RealVector MP_ (continuousDesignUpperBnds)
- static RealVector MP_ (continuousDesignVars)
- static RealVector MP_ (continuousDesignScales)
- static RealVector MP_ (continuousIntervalUncVars)
- static RealVector MP_ (continuousStateLowerBnds)
- static RealVector MP_ (continuousStateUpperBnds)
- static RealVector MP_ (continuousStateVars)
- static RealVector MP_ (discreteDesignSetRealVars)
- static RealVector MP_ (discreteStateSetRealVars)
- static RealVector MP_ (discreteUncSetRealVars)
- static RealVector MP_ (frechetUncBetats)
- static RealVector MP_ (frechetUncVars)
- static RealVector MP_ (geometricUncProbPerTrial)
- static RealVector MP_ (gumbelUncBetats)
- static RealVector MP_ (gumbelUncVars)
- static RealVector MP_ (histogramBinUncVars)
- static RealVector MP_ (histogramPointRealUncVars)
- static RealVector MP_ (linearEqConstraintCoeffs)
- static RealVector MP_ (linearEqScales)
- static RealVector MP_ (linearEqTargets)
- static RealVector MP_ (linearIneqConstraintCoeffs)
- static RealVector MP_ (linearIneqLowerBnds)
- static RealVector MP_ (linearIneqUpperBnds)
- static RealVector MP_ (linearIneqScales)
- static RealVector MP_ (negBinomialUncProbPerTrial)
- static RealVector MP_ (normalUncLowerBnds)
- static RealVector MP_ (normalUncMeans)
- static RealVector MP_ (normalUncUpperBnds)
- static RealVector MP_ (normalUncVars)
- static RealVector MP_ (triangularUncModes)
- static RealVector MP_ (triangularUncVars)
- static RealVector MP_ (uniformUncVars)
- static RealVector MP_ (weibullUncVars)
- static RealVector VP_ (ddsr)
12.1. DAKOTA NAMESPACE REFERENCE

- static RealVector $\text{VP}_\text{r}$ (dssr)
- static RealVector $\text{VP}_\text{r}$ (dusr)
- static RealVector $\text{VP}_\text{r}$ (ClLib)
- static RealVector $\text{VP}_\text{r}$ (ClUub)
- static RealVector $\text{VP}_\text{r}$ (Clp)
- static RealVector $\text{VP}_\text{r}$ (Dlp)
- static RealVector $\text{VP}_\text{r}$ (DSIp)
- static RealVector $\text{VP}_\text{r}$ (DSSp)
- static RealVector $\text{VP}_\text{r}$ (DSRp)
- static RealVector $\text{VP}_\text{r}$ (hba)
- static RealVector $\text{VP}_\text{r}$ (hbo)
- static RealVector $\text{VP}_\text{r}$ (hbc)
- static RealVector $\text{VP}_\text{r}$ (hpic)
- static RealVector $\text{VP}_\text{r}$ (hpsc)
- static RealVector $\text{VP}_\text{r}$ (hprr)
- static RealVector $\text{VP}_\text{r}$ (hprrc)
- static RealVector $\text{VP}_\text{r}$ (ucm)
- static String $\text{MP}_\text{r}$ (idVariables)
- static StringArray $\text{MP}_\text{r}$ (continuousDesignLabels)
- static StringArray $\text{MP}_\text{r}$ (continuousDesignScaleTypes)
- static StringArray $\text{MP}_\text{r}$ (continuousStateLabels)
- static StringArray $\text{MP}_\text{r}$ (continuousStateScaleTypes)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignRangeLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetIntLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetIntLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetIntLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetRealLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetRealLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteDesignSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteUncSetIntLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteUncSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteUncSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteUncSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (discreteUncSetStrLabels)
- static StringArray $\text{MP}_\text{r}$ (histogramPointStrUncVars)
- static StringArray $\text{MP}_\text{r}$ (linearEqScaleTypes)
- static StringArray $\text{MP}_\text{r}$ (linearIneqScaleTypes)
- static StringArray $\text{VP}_\text{r}$ (hpsa)
- static StringArray $\text{VP}_\text{r}$ (ddss)
- static StringArray $\text{VP}_\text{r}$ (duss)
- static StringArray $\text{VP}_\text{r}$ (dsss)
- static BitArray $\text{MP}_\text{r}$ (discreteDesignSetIntCat)
- static BitArray $\text{MP}_\text{r}$ (discreteDesignSetRealCat)
- static BitArray $\text{MP}_\text{r}$ (discreteStateSetIntCat)
- static BitArray $\text{MP}_\text{r}$ (discreteStateSetRealCat)
- static BitArray $\text{MP}_\text{r}$ (discreteUncSetIntCat)
- static BitArray $\text{MP}_\text{r}$ (discreteUncSetRealCat)
- static Var $\text{brv}$ MP2s (betaUncAlphas, 0.)
- static Var_brv MP2s (betaUncBetas, 0.)
- static Var_brv MP2s (exponentialUncBetas, 0.)
- static Var_brv MP2s (exponentialUncVars, 0.)
- static Var_brv MP2s (frechetUncAlphas, 2.)
- static Var_brv MP2s (gammaUncAlphas, 0.)
- static Var_brv MP2s (gammaUncBetas, 0.)
- static Var_brv MP2s (gammaUncVars, 0.)
- static Var_brv MP2s (gumbelUncAlphas, 0.)
- static Var_brv MP2s (lognormalUncErrFacts, 1.)
- static Var_brv MP2s (lognormalUncLambdas, 0.)
- static Var_brv MP2s (lognormalUncLowerBnds, 0.)
- static Var_brv MP2s (lognormalUncMeans, 0.)
- static Var_brv MP2s (lognormalUncStdDevs, 0.)
- static Var_brv MP2s (lognormalUncUpperBnds, std::numeric_limits<Real>::infinity())
- static Var_brv MP2s (lognormalUncVars, 0.)
- static Var_brv MP2s (lognormalUncZetas, 0.)
- static Var_brv MP2s (loguniformUncLowerBnds, 0.)
- static Var_brv MP2s (loguniformUncUpperBnds, std::numeric_limits<Real>::infinity())
- static Var_brv MP2s (loguniformUncVars, 0.)
- static Var_brv MP2s (normalUncStdDevs, 0.)
- static Var_brv MP2s (poissonUncLambdas, 0.)
- static Var_brv MP2s (triangularUncLowerBnds, std::numeric_limits<Real>::infinity())
- static Var_brv MP2s (triangularUncUpperBnds, std::numeric_limits<Real>::infinity())
- static Var_brv MP2s (uniformUncLowerBnds, std::numeric_limits<Real>::infinity())
- static Var_brv MP2s (uniformUncUpperBnds, std::numeric_limits<Real>::infinity())
- static Var_brv MP2s (weibullUncAlphas, 0.)
- static Var_brv MP2s (weibullUncBetas, 0.)
- static Var_biv MP2s (binomialUncNumTrials, 0)
- static Var_biv MP2s (binomialUncVars, 0)
- static Var_biv MP2s (geometricUncVars, 0)
- static Var_biv MP2s (hyperGeomUncNumDrawn, 0)
- static Var_biv MP2s (hyperGeomUncSelectedPop, 0)
- static Var_biv MP2s (hyperGeomUncTotalPop, 0)
- static Var_biv MP2s (hyperGeomUncVars, 0)
- static Var_biv MP2s (negBinomialUncNumTrials, 0)
- static Var_biv MP2s (negBinomialUncVars, 0)
- static Var_biv MP2s (poissonUncVars, 0)
- static Var_mp_type Vtype (varsDomain, MIXED_DOMAIN)
- static Var_mp_type Vtype (varsDomain, RELAXED_DOMAIN)
- static Var_mp_type Vtype (varsView, ALL_VIEW)
- static Var_mp_type Vtype (varsView, DESIGN_VIEW)
- static Var_mp_type Vtype (varsView, UNCERTAIN_VIEW)
- static Var_mp_type Vtype (varsView, ALEATORY_UNCERTAIN_VIEW)
- static Var_mp_type Vtype (varsView, EPISTEMIC_UNCERTAIN_VIEW)
- static Var_mp_type Vtype (varsView, STATE_VIEW)
void flatten_num_array (const std::vector< ContainerT > &input_array, IntArray &outia)

Free convenience function that flatten sizes of an array of std containers; takes an array of containers and returns an IntArray containing the sizes of each container in the input array. Note: Did not specialize for vector<RealVector>
as no current use cases.

void dn2f_ (int *n, int *p, Real *x, Calcrj, int *iv, int *liv, int *lv, Real *v, int *ui, void *ur, Vf)
void dn2fb_ (int *n, int *p, Real *x, Real *b, Calcrj, int *iv, int *liv, int *lv, Real *v, int *ui, void *ur, Vf)
void dn2gb_ (int *n, int *p, Real *x, Real *b, Calcrj, Calcrj, int *iv, int *liv, int *lv, Real *v, int *ui, void *ur, Vf)
void divset_ (int *, int *, int *, int *, Real *)
double dr7mdc_ (int *)
static void Rswapchk (NI2Misc *q)
static int hasnaninf (const double *d, int n)
NLPQLPOptimizer * new_NLPQLPOptimizer (ProblemDescDB &problem_db, Model &model)
NLPQLPOptimizer * new_NLPQLPOptimizer (Model &model)
NOWPACOptimizer * new_NOWPACOptimizer (ProblemDescDB &problem_db, Model &model)
NOWPACOptimizer * new_NOWPACOptimizer (Model &model)
NPSOLOptimizer * new_NPSOLOptimizer (ProblemDescDB &problem_db)
NPSOLOptimizer * new_NPSOLOptimizer1 (Model &model)
NPSOLOptimizer * new_NPSOLOptimizer2 (Model &model, const int &derivative_level, const Real &conv_tol)
NPSOLOptimizer * new_NPSOLOptimizer3 (const RealVector &initial_point, const RealVector &var_,
lower_bnds, const RealVector &var_upper_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_
ineq_lower_bnds, const RealVector &lin_ineq_upper_bnds, const RealMatrix &lin_eq, const RealVector &lin_
ineq_targets, const RealVector &nonlin_ineq_lower_bnds, const RealVector &nonlin_ineq_upper_
bnds, const RealVector &nonlin_eq_targets, void(*user_obj_eval)(int &, int &, double *, double &,
double *, int &), void(*user_con_eval)(int &, int &, int &, int &, int *, double *, double *, double *,
int &), const int &derivative_level, const Real &conv_tol)
NPSOLOptimizer * new_NPSOLOptimizer (ProblemDescDB &problem_db, Model &model)
NPSOLOptimizer * new_NPSOLOptimizer (Model &model)
NPSOLOptimizer * new_NPSOLOptimizer (Model &model, const int &, const Real &)
NPSOLOptimizer * new_NPSOLOptimizer (const RealVector &initial_point, const RealVector &var_,
lower_bnds, const RealVector &var_upper_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_
ineq_lower_bnds, const RealVector &lin_ineq_upper_bnds, const RealMatrix &lin_eq, const RealVector &lin_
ineq_targets, const RealVector &nonlin_ineq_lower_bnds, const RealVector &nonlin_ineq_upper_
bnds, const RealVector &nonlin_eq_targets, void(*user_obj_eval)(int &, int &, double *, double &,
double *, int &), void(*user_con_eval)(int &, int &, int &, int &, int *, double *, double *, double *,
int &), const int &derivative_level, const Real &conv_tol)
void start_dakota_heartbeat (int)
void dak_sigcatch (int sig)
MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, ParallelLevel &pl)
MPIUnpackBuffer extraction operator for ParallelLevel. Calls read(MPIUnpackBuffer&).
MPIPackBuffer & operator<< (MPIPackBuffer &s, const ParallelLevel &pl)
MPIPackBuffer insertion operator for ParallelLevel. Calls write(MPIPackBuffer&).
std::istream & operator>> (std::istream &s, ParamResponsePair &pair)
std::istream extraction operator for ParamResponsePair
• std::ostream & operator<< (std::ostream &s, const ParamResponsePair &pair)
  std::ostream insertion operator for ParamResponsePair.
• MPIUnpackBuffer & operator>>(MPIUnpackBuffer &s, ParamResponsePair &pair)
  MPIUnpackBuffer extraction operator for ParamResponsePair.
• MPIPackBuffer & operator<<(MPIPackBuffer &s, const ParamResponsePair &pair)
  MPIPackBuffer insertion operator for ParamResponsePair.
• bool operator==(const ParamResponsePair &pair1, const ParamResponsePair &pair2)
  equality operator for ParamResponsePair.
• bool operator!=(const ParamResponsePair &pair1, const ParamResponsePair &pair2)
  inequality operator for ParamResponsePair.
• static void *binsearch (void *kw, size_t kwsiz, size_t n, const char *key)
• static const char *Begins (const String &entry_name, const char *s)
• static void Bad_name (String entry_name, const char *where)
• static void Locked_db ()
• static void Null_rep (const char *who)
• static void Null_rep1 (const char *who)
• MPIUnpackBuffer & operator>>(MPIUnpackBuffer &s, ProgramOptions &progopt)
  MPIUnpackBuffer extraction operator.
• MPIPackBuffer & operator<<(MPIPackBuffer &s, const ProgramOptions &progopt)
  MPIPackBuffer insertion operator.
• bool set_compare (const ParamResponsePair &database_pr, const ActiveSet &search_set)
  search function for a particular ParamResponsePair within a PRPList based on ActiveSet content (request vector and derivative variables vector).
• bool id_vars_exact_compare (const ParamResponsePair &database_pr, const ParamResponsePair &search_pr)
  search function for a particular ParamResponsePair within a PRPMultiIndex.
• std::size_t hash_value (const ParamResponsePair &prp)
  hash_value for ParamResponsePairs stored in a PRPMultiIndex.
• PRPCacheHIter hashedCacheBegin (PRPCache &prp_cache)
  hashed definition of cache begin.
• PRPCacheHIter hashedCacheEnd (PRPCache &prp_cache)
  hashed definition of cache end.
• PRPQueueHIter hashedQueueBegin (PRPQueue &prp_queue)
  hashed definition of queue begin.
• PRPQueueHIter hashedQueueEnd (PRPQueue &prp_queue)
  hashed definition of queue end.
• PRPCacheHIter lookup_by_val (PRPMultiIndexCache &prp_cache, const ParamResponsePair &search_pr)
  find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.
• PRPCacheHIter lookup_by_val (PRPMultiIndexCache &prp_cache, const String &search_interface_id, const Variables &search_vars, const ActiveSet &search_set)
  find a ParamResponsePair within a PRPMultiIndexCache based on the interface id, variables, and ActiveSet search data.
• PRPCacheOIter lookup_by_nearby_val (PRPMultiIndexCache &prp_cache, const String &search_interface_id, const Variables &search_vars, const ActiveSet &search_set, Real tol)
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- PRPCacheOIter lookup_by_ids (PRPMultiIndexCache &prp_cache, const IntStringPair &search_ids)
  find a ParamResponsePair within a PRPMultiIndexCache based on search_ids (i.e. std::pair<eval_id,interface_id>) search data
- PRPCacheOIter lookup_by_ids (PRPMultiIndexCache &prp_cache, const IntStringPair &search_ids, const ParamResponsePair &search_pr)
- PRPQueueHIter lookup_by_val (PRPMultiIndexQueue &prp_queue, const ParamResponsePair &search_pr)
  find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.
- PRPQueueHIter lookup_by_val (PRPMultiIndexQueue &prp_queue, const String &search_interface_id, const Variables &search_vars, const ActiveSet &search_set)
  find a ParamResponsePair within a PRPMultiIndexQueue based on interface id, variables, and ActiveSet search data
- PRPQueueOIter lookup_by_eval_id (PRPMultiIndexQueue &prp_queue, int search_id)
  find a ParamResponsePair within a PRPMultiIndexQueue based on search_id (i.e. integer eval_id) search data
- void print_usage (std::ostream &s)
  print restart utility help message
- void print_restart (StringArray pos_args, String print_dest)
  print a restart file
- void print_restart_pdb (StringArray pos_args, String print_dest)
  print a restart file (PDB format)
- void print_restart_tabular (StringArray pos_args, String print_dest, unsigned short tabular_format, int tabular_precision)
  print a restart file (tabular format)
- void read_neutral (StringArray pos_args)
  read a restart file (neutral file format)
- void repair_restart (StringArray pos_args, String identifier_type)
  repair a restart file by removing corrupted evaluations
- void concatenate_restart (StringArray pos_args)
  concatenate multiple restart files
- static HANDLE * wait_setup (std::map< pid_t, int > *M, size_t *pn)
- static int wait_for_one (size_t n, HANDLE *h, int req1, size_t *pi)
- void gauss_legendre_pts_wts_1D (int level, RealVector &result_0, RealVector &result_1)
- void lagrange_interpolation_1d (const RealVector &samples, const RealVector &abscissa, const RealVector &values, RealVector &result)
- void kronecker_product_2d (const RealMatrix &matrix1, const RealMatrix &matrix2, RealMatrix &matrix)
- void get_chebyshev_points (int order, RealVector &points)
- void chebyshev_derivative_matrix (int order, RealMatrix &derivative_matrix, RealVector &points)
- int salinas_main (int argc, char *argv[], MPI_Comm *comm)
  subroutine interface to SALINAS simulation code
- std::string get_cwd_str ()
- std::vector< std::string > get_pathext ()
- bool contains (const bfs::path &dir_path, const std::string &file_name, boost::filesystem::path &complete_filepath)
CHAPTER 12. NAMESPACE DOCUMENTATION

Variables

- PRPCache data_pairs
  contains all parameter/response pairs.
- double PI = boost::math::constants::pi<>()
  constant pi
- double HALF_LOG_2PI = std::log(2.0*PI)/2.0
  constant log(2*pi)/2.0
- short abort_mode = ABORT_EXITs
  by default Dakota exits or calls MPI_Abort on errors
- std::ostream *dakota_cout = &std::cout
  DAKOTA stdout initially points to < std::cout, but may be redirected to a tagged ofstream if there are < concurrent iterators.
- std::ostream *dakota_cerr = &std::cerr
  DAKOTA stderr initially points to < std::cerr, but may be redirected to a tagged ofstream if there are < concurrent iterators.
- ResultsManager iterator_results_db
  Global results database for iterator results.
- int write_precision = 10
  used in ostringstream data output functions < (restart_util.cpp overrides default value)
- MPIManager dummy_mpi_mgr
  dummy MPIManager for ref initialization
- ProgramOptions dummy_prg_opt
  dummy ProgramOptions for ref initialization
- OutputManager dummy_out_mgr
  dummy OutputManager for ref initialization
- ParallelLibrary dummy_lib
  dummy ParallelLibrary for ref initialization
- ProblemDescDB dummy_db
  dummy ProblemDescDB for ref initialization
- int mc_ptr_int = 0
  global pointer for ModelCenter API
- int dc_ptr_int = 0
  global pointer for ModelCenter eval DB
- ProblemDescDB *Dak_pddb
  set by ProblemDescDB, for use in parsing
- const size_t NPOS = ~size_t(0)
  special value returned by index() when entry not found
- const double BIG_REAL_BOUND = 1.0e+30
  bound beyond which constraints are considered inactive
- Interface dummy_interface
  dummy Interface object used for mandatory
  < reference initialization or default virtual < function return by reference when a real < Interface instance is unavailable
- Model dummy_model
12.1. DAKOTA NAMESPACE REFERENCE

dummy Model object used for mandatory reference
< initialization or default virtual function < return by reference when a real Model instance < is unavailable

- Iterator dummy_iterator
  dummy Iterator object used for mandatory
  < reference initialization or default virtual < function return by reference when a real < Iterator instance is unavailable

- Dakota_funcs * DF
- Dakota_funcs DakFuncs0
- const char * FIELD_NAMES [ ]
- const int NUMBER_OF_FIELDS = 23
- static const int MPI_COMM_WORLD = 1
- static const int MPI_COMM_NULL = 0
- static const int MPI_COMM_SELF = 92
- static const int MPI_ANY_TAG = -1
- static void * MPI_REQUEST_NULL = NULL
- FILE * nidrin
- const size_t NIDR_MAX_ERROR_LEN = 8192

maximum error length is roughly 100 lines at 80 char; using fixed error length instead of investing in converting to vsnprintf (C++11)

- static const char * aln_scaletypes [ ] = { "auto", "log", "none", 0 }
- static Var_uinfo CAUVlbl [CAUVar_Nkinds]
- static Var_uinfo DAUIVLbl [DAUIVar_Nkinds]
- static Var_uinfo DAUSVLbl [DAUSVar_Nkinds]
- static Var_uinfo CEUVlbl [CEUVar_Nkinds]
- static Var_uinfo DEUIVLbl [DEUIVar_Nkinds]
- static Var_uinfo DEUSVLbl [DEUSVar_Nkinds]
- static Var_uinfo DEURVLbl [DEURVar_Nkinds]
- static Var_uinfo DiscSetLbl [DiscSetVar_Nkinds]
- static VarLabelChk DesignAndStateLabelsCheck [ ]

Variables label array designations for design and state. All non-uncertain variables need to be in this array. Used in check_variables_node to check lengths and make_variable_defaults to build labels.

- static VLreal VLUncertainReal [NUM_UNC_REAL_CONT]

Variables labels/bounds/values check array for real-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., CAUVlbl, with the contiguous container in which they are stored.

- static VLint VLUncertainInt [NUM_UNC_INT_CONT]

Variables labels/bounds/values check array for integer-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUIVLbl, with the contiguous container in which they are stored.

- static VLstr VLUncertainStr [NUM_UNC_STR_CONT]

Variables labels/bounds/values check array for string-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUSVLbl, with the contiguous container in which they are stored.

- static int VLR_aleatory [NUM_UNC_REAL_CONT] = { 1, 0, 1, 0 }

which uncertain real check array containers are aleatory (true = 1)

- static int VLI_aleatory [NUM_UNC_INT_CONT] = { 1, 0 }
which uncertain integer check array containers are aleatory (true = 1)

- static int VLS_aleatory[NUM_UNC_STR_CONT] = { 1, 0 }

which uncertain string check array containers are aleatory (true = 1)

- static Var_check var_mp_check_cv [ ]
- static Var_check var_mp_check_dset [ ]
- static Var_check var_mp_check_cau [ ]
- static Var_check var_mp_check_daui [ ]
- static Var_check var_mp_check_daus [ ]
- static Var_check var_mp_check_dau [ ]
- static Var_check var_mp_check_dcv [ ]
- static Var_check var_mp_check_dceu [ ]
- static Var_check var_mp_check_deui [ ]
- static Var_check var_mp_check_deus [ ]
- static Var_check var_mp_check_deur [ ]
- static Var_rcheck var_mp_ebound [ ]

This is used within check_variables_node(): Var_RealBoundIPCheck() is applied to validate bounds and initial points.

- static Var_rcheck var_mp_drange [ ]

This is used in check_variables_node(): Var_IntBoundIPCheck() is applied to validate bounds and initial points, and in make_variable_defaults(): Vgen_* is called to infer bounds.

- static time t_start_time
- const char * SCI_FIELD_NAMES [ ]
- const int SCI_NUMBER_OF_FIELDS = 26
- const int LARGE_SCALE = 100

a (perhaps arbitrary) definition of large scale; choose a large-scale algorithm if numVars >= LARGE_SCALE

- const double POW_VAL = 1.0

offset used text book exponent: 1.0 is nominal, 1.4 used for B&B testing

- const String LEV_REF = "Dakota"

levenshtein.distance computes the distance between its argument and this

12.1.1 Detailed Description

The primary namespace for DAKOTA. The Dakota namespace encapsulates the core classes of the DAKOTA framework and prevents name clashes with third-party libraries from methods and packages. The C++ source files defining these core classes reside in Dakota/src as *.cpp.

Work directory TODO
Doc: we will search for drivers in PATH, workdir (.), RUNDIR
Remove legacy utilities (once concepts migrated)

- In general review cases with race conditions such as single dir getting created / removed for each eval.
- Verify creation/removal in parallel runs (eval_comm_rank 0?): are there scenarios where we should create once ahead of time?
- Enforce tagging when async is possible
- Challenge of shared vs. distinct filesystems
- Verify template files exist at parse and that workdir parent exists
• Verify behavior when directory exists
• Allow recursive copy to descend to overwrite leaf nodes when directories already exist
• Old code setting permissions mask 0700
• Workdir with multiple analysis components (per analysis)
• Workdirs shared for each unique concurrent eval (not per eval ID)
• Evaluate environment variables
• How to manage drivers that want just param names in the work dir?!? I think arg_adjust is removing the directory args that aren’t needed.
• Consider making the class members for directories and files bfs::paths
• Behavior of file_save when directory not saved
• Error checking: directory was created directory path is a directory directory has rwx for user population worked try/catch around all fs operations
• Verify correct handling of relative vs. absolute files/dirs
• Enforce that first argument must be an executable program for all drivers; at least for fork
• Historical behaviors / features to consider Template dirs on PATH: likely no longer
  Allowed FOO=zorch and would set that in the environment; could allow separate env var specification; otherwise likely remove
• TODO: pass environment to exec as separate pointer

TESTING NEEDS
• Allow nested quotes in driver, at least one level: analysis_driver = ‘ad.sh “-opt foo -opt1 goo”’ p.in.1 r.out.1
• Env vars will be carried along for now, not expanded before eval; set some helpful env vars before the eval.

12.1.2 Typedef Documentation

typedef bmi::multi_index_container< Dakota::ParamResponsePair, bmi::indexed_by< bmi::ordered_non_unique< bmi::tag< ordered >, bmi::const_mem_fun< Dakota::ParamResponsePair, const IntStringPair&, &Dakota::ParamResponsePair::eval_interface_ids > >, bmi::hashed_non_unique< bmi::tag< hashed >, bmi::identity< Dakota::ParamResponsePair >, partial_prp_hash, partial_prp_equality > > > PRPMultiIndexCache

Boost Multi-Index Container for globally caching ParamResponsePairs.

For a global cache, both evaluation and interface id’s are used for tagging ParamResponsePair records.

typedef bmi::multi_index_container< Dakota::ParamResponsePair, bmi::indexed_by< bmi::ordered_unique< bmi::tag< ordered >, bmi::const_mem_fun< Dakota::ParamResponsePair, int, &Dakota::ParamResponsePair::eval_id > >, bmi::hashed_non_unique< bmi::tag< hashed >, bmi::identity< Dakota::ParamResponsePair >, partial_prp_hash, partial_prp_equality > > > PRPMultiIndexQueue

Boost Multi-Index Container for locally queueing ParamResponsePairs.

For a local queue, interface id’s are expected to be consistent, such that evaluation id’s are sufficient for tracking particular evaluations.
12.1.3 Enumeration Type Documentation

anonymous enum
Sub-methods, including sampling, inference algorithm, opt algorithm types.

Enumerator

  SUBMETHOD_COLLABORATIVE  Type of hybrid meta-iterator:

12.1.4 Function Documentation

CommandShell & flush ( CommandShell & shell )
convenient shell manipulator function to "flush" the shell
  global convenience function for manipulating the shell; invokes the class member flush function.
  References CommandShell::flush().
  Referenced by SysCallApplicInterface::spawn_analysis_to_shell(), SysCallApplicInterface::spawn_evaluation_to_shell(), SysCallApplicInterface::spawn_input_filter_to_shell(), and SysCallApplicInterface::spawn_output_filter_to_shell().

void abort_throw_or_exit ( int dakota_code )
throw or exit depending on abort_mode
  Throw a Boost system_error or call std::exit, with (256 + dakota_code), where dakota_code < 0
  RATIONALE: Avoid common "standard" exit codes and signals (signum.h) as well as uncaught signals / uncatchable SIGKILL which return 128
  • <signum> on Linux = [129, 192]
  Return a value in [0,255] since some operating systems only return the 8 least significant bits, leaves [193, 255] for Dakota. This should make return codes consistent cross-platform.
  References abort_mode.
  Referenced by abort_handler(), and ParallelLibrary::abort_helper().

void register_signal_handlers ( )
Tie various signal handlers to Dakota’s abort_handler function.
  Global function to register signal handlers at top-level.
  References abort_handler().
  Referenced by main().

void mpi_debug_hold ( )
Global function to hold Dakota processes to help with MPI debugging.
  See details in code for details, depending on MPI implementation in use.
  Referenced by main().

T Dakota::abort_handler_t ( int code )
Templatized abort_handler_t method that allows for convenient return from methods that otherwise have no sensible return from error clauses. Usage: MyType& method() { return abort_handler<MyType&>(-1); }
  References abort_handler().
void svd ( RealMatrix & matrix, RealVector & singular_vals, RealMatrix & v_trans, bool compute_vectors = true )

Compute the SVD of an arbitrary matrix A = USV^T.

Uses Teuchos::LAPACK.GESVD() to compute the singular value decomposition, overwriting A with the left singular vectors U (or destroying A if compute_vectors = false); optionally returns right singular vectors in v_trans.

References abort_handler().

Referenced by NonDBayesCalibration::build_model_discrepancy(), PebblBranchSub::candidateSolution(), NestedModel::cdiv_index_map(), NestedModel::cdsv_index_map(), ActiveSubspaceModel::compute_svd(), ActiveSubspaceModel::computeBingLiCriterion(), ActiveSubspaceModel::computeConstantineMetric(), Variables::continuous_variable_id(), Variables::continuous_variable_type(), Variables::continuous_variable_labels(), Variables::continuous_variable_types(), Variables::continuous_variable_types(), SharedVariablesData::copy(), NestedModel::cv_index_map(), Model::discrete_int_sets(), Variables::discrete_int_variable_label(), Variables::discrete_int_variable_labels(), Variables::discrete_int_variable_types(), Variables::discrete_int_variable_types(), Variables::discrete_real_variable_label(), Variables::discrete_real_variable_labels(), Variables::discrete_real_variable_types(), Variables::discrete_real_variable_types(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Variables::discrete_string_variable_label(), Variables::discrete_string_variable_labels(), Variables::discrete_string_variable_type(), Variables::discrete_string_variable_types(), ParamStudy::distribute(), NestedModel::div_index_map(), NestedModel::drv_index_map(), NestedModel::dsv_index_map(), DataTransformModel::get_hyperparam_vc_index(), Variables::inactive_continuous_variable_ids(), Variables::inactive_continuous_variable_labels(), Variables::inactive_continuous_variable_types(), Variables::inactive_continuous_variable_types(), Variables::inactive_continuous_variable_types(), Variables::inactive_continuous_variable_types(), Variables::inactive_continuous_variable_types(), Variables::inactive_continuous_variable_types(), DataTransformModel::init_continuous_vars(), RecastModel::init_variables(), NonD::NonD, Optimizer::Optimizer(), SensAnalysisGlobal::partial_corr(), ParamStudy::pre_run(), ProbabilityTransformModel::ProbabilityTransformModel(), Constraints::reshape(), NonD::resize(), singular_values(), NonD::size(), PebblBranchSub::splitComputation(), NonD::transform_model(), ReducedBasis::update_svd(), DataTransformModel::variables_expand(), RandomFieldModel::variables_resize(), AdaptedBasisModel::variables_resize(), and ActiveSubspaceModel::variables_resize().

int qr ( RealMatrix & A )

Compute an in-place QR factorization A = QR.

Uses Teuchos::LAPACK.GEQRF() to compute the QR decomposition, overwriting A with the transformations and R.

References abort_handler().

Referenced by SensAnalysisGlobal::partial_corr().

int qr_rsolve ( const RealMatrix & q,r, bool transpose, RealMatrix & rhs )

Perform a multiple right-hand sides Rinv * rhs solve using the R from a qr factorization.

Returns info > 0 if the matrix is singular

Uses Teuchos::LAPACK.TRTRS() to perform a triangular backsolve

References abort_handler().

Referenced by SensAnalysisGlobal::partial_corr().

bool Dakota::operator!= ( const ActiveSet & set1, const ActiveSet & set2 ) [inline]

inequality operator for ActiveSet
bool Dakota::operator== ( const Model & m1, const Model & m2 ) [inline]
equality operator for Envelope is true if same letter instance
equality operator (detect same letter instance)
References Model::modelRep.

bool Dakota::operator!= ( const Model & m1, const Model & m2 ) [inline]
inequality operator for Envelope is true if different letter instance
inequality operator (detect different letter instances)
References Model::modelRep.

bool Dakota::operator!= ( const Response & resp1, const Response & resp2 ) [inline]
inequality operator for Response
inequality operator

bool Dakota::operator!= ( const Variables & vars1, const Variables & vars2 ) [inline]
inequality operator for Variables
strict inequality operator

void Dakota::write_ordered ( std::ostream & s, const SizetArray & comp_totals, const Teuchos::SerialDenseVector<OrdinalType, ScalarType1> & c_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType2> & di_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType3> & ds_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType4> & dr_vector ) [inline]
free function to write Variables data vectors in input spec ordering
written for arbitrary types, but typical use will be ScalarType1 = Real, ScalarType2 = int, ScalarType3 = string,
and ScalarType4 = int or Real.
Referenced by ParamStudy::pre_run().

void Dakota::write_ordered ( std::ostream & s, const SizetArray & comp_totals, const Teuchos::SerialDenseVector<OrdinalType, ScalarType1> & c_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType2> & di_vector, const Teuchos::SerialDenseVector<OrdinalType, ScalarType4> & dr_vector ) [inline]
free function to write Variables data vectors in input spec ordering
written for arbitrary types, but typical use will be ScalarType1 = Real, ScalarType2 = int, ScalarType3 = string,
and ScalarType4 = int or Real.

void copy_field_data ( const RealVector & fn_vals, RealMatrix & fn_grad, const RealSymMatrixArray & fn_hess, size_t offset, size_t num_fns, Response & response )
This assumes the source gradient/Hessian are size less or equal to the destination response, and that the leading
part is to be populated.
References Response::active_set_request_vector(), Response::function_gradient_view(), Response::function_hessian_view(), and Response::function_value().
Referenced by ExperimentData::scale_residuals().
void Dakota::copy_field_data ( const RealVector & fn_vals, RealMatrix & fn_grad, const
RealSymMatrixArray & fn_hess, size_t offset, size_t num_fns, short total_asv, Response & response )

This assumes the source gradient/Hessian are size less or equal to the destination response, and that the leading
part is to be populated.

References Response::function_gradient_view(), Response::function_hessian_view(), and Response::function_value().

void symmetric_eigenvalue_decomposition ( const RealSymMatrix & matrix, RealVector & eigenvalues,
RealMatrix & eigenvectors )

Computes the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A.

Eigenvalues are returned in ascending order.

References symmetric_eigenvalue_decomposition().

Referenced by NonDBayesCalibration::get_positive_definite_covariance_from_hessian(), and symmetric_eigenvalue_decomposition().

Real Dakota::getdist ( const RealVector & x1, const RealVector & x2 )

Gets the Euclidean distance between x1 and x2.

Referenced by mindist(), and mindistidx().

Real Dakota::mindist ( const RealVector & x, const RealMatrix & xset, int except )

Returns the minimum distance between the point x and the points in the set xset (compares against all points in
xset except point "except"): if except is not needed, pass 0.

References getdist().

Referenced by getRmax().

Real Dakota::mindistidx ( const RealVector & x, const RealMatrix & xset, const IntArray & indx )

Gets the min distance between x and points in the set xset defined by the nindx values in indx.

References getdist().

Referenced by GaussProcApproximation::pointsel_add_sel().

Real Dakota::getRmax ( const RealMatrix & xset )

Gets the maximum of the min distance between each point and the rest of the set.

References mindist().

Referenced by GaussProcApproximation::pointsel_add_sel().

int Dakota::start_grid_computing ( char * analysis_driver_script, char * params_file, char * results_file )

sample function prototype for launching grid computing

int Dakota::stop_grid_computing ( )

sample function prototype for terminating grid computing

int Dakota::perform_analysis ( char * iteration_num )

sample function prototype for submitting a grid evaluation
string Dakota::asstring ( const T & val )

Creates a string from the argument val using an ostringstream.

This only gets used in this file and is only ever called with ints so no error checking is in place.

Parameters

| val | The value of type T to convert to a string. |

Returns

The string representation of val created using an ostringstream.

Referenced by JEGAOptimizer::LoadTheConstraints().

void start_dakota_heartbeat ( int seconds )

Heartbeat function provided by dakota_filesystem_utils; pass output interval in seconds, or -1 to use DAKOTA_HEARTBEAT

Referenced by OutputManager::OutputManager().

bool Dakota::operator==( const ParamResponsePair & pair1, const ParamResponsePair & pair2 ) [inline]

equality operator for ParamResponsePair

equality operator

References ParamResponsePair::evalInterfaceIds, ParamResponsePair::prpResponse, and ParamResponsePair::prpVariables.

bool Dakota::operator!=( const ParamResponsePair & pair1, const ParamResponsePair & pair2 ) [inline]

inequality operator for ParamResponsePair

inequality operator

bool Dakota::set_compare ( const ParamResponsePair & database_pr, const ActiveSet & search_set ) [inline]

search function for a particular ParamResponsePair within a PRPList based on ActiveSet content (request vector and derivative variables vector)

a global function to compare the ActiveSet of a particular database_pr (presumed to be in the global history list) with a passed in ActiveSet (search_set).

References ParamResponsePair::active_set(), ActiveSet::derivative_vector(), and ActiveSet::request_vector().

Referenced by lookup_by_val().

bool Dakota::id_vars_exact_compare ( const ParamResponsePair & database_pr, const ParamResponsePair & search_pr ) [inline]

search function for a particular ParamResponsePair within a PRPMultiIndex

a global function to compare the interface id and variables of a particular database_pr (presumed to be in the global history list) with a passed in key of interface id and variables provided by search_pr.

References ParamResponsePair::interface_id(), and ParamResponsePair::variables().

Referenced by partial_prp_equality::operator().
PRPCacheHIter Dakota::lookup by_val ( PRPMultiIndexCache & prp_cache, const ParamResponsePair & search_pr ) [inline]

find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.

Lookup occurs in two steps: (1) PRPMultiIndexCache lookup based on strict equality in interface id and variables, and (2) set_compare() post-processing based on ActiveSet subset logic.

References ParamResponsePair::active_set(), and set_compare().

Referenced by NonDQUESOBayesCalibration::aggregate_acceptance_chain(), NonDDREAMBayesCalibration::archive_acceptance_chain(), Model::db_lookup(), ApplicationInterface::duplication_detect(), SurrBasedLocalMinimizer::find_response(), Minimizer::local_recast_retrieve(), lookup_by_val(), SNLLLeastSq::post_run(), PebbldMinimizer::print_results(), SurrBasedMinimizer::print_results(), Optimizer::print_results(), DiscrepancyCorrection::search_db(), and NonDLocalReliability::update_mpp_search_data().

PRPQueueHIter Dakota::lookup by_val ( PRPMultiIndexQueue & prp_queue, const ParamResponsePair & search_pr ) [inline]

find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.

Lookup occurs in two steps: (1) PRPMultiIndexQueue lookup based on strict equality in interface id and variables, and (2) set_compare() post-processing based on ActiveSet subset logic.

References ParamResponsePair::active_set(), and set_compare().

void print_restart ( StringArray pos_args, String print_dest )

print a restart file

Usage: "dakota_restart_util print dakota.rst"
"dakota_restart_util to_neutral dakota.rst dakota.neu"

Prints all evals. in full precision to either stdout or a neutral file. The former is useful for ensuring that duplicate detection is successful in a restarted run (e.g., starting a new method from the previous best), and the latter is used for translating binary files between platforms.

References abort_handler(), ParamResponsePair::eval_id(), ParamResponsePair::write_annotated(), and write_precision.

Referenced by main().

void print_restart_pdb ( StringArray pos_args, String print_dest )

print a restart file (PDB format)

Usage: "dakota_restart_util to_pdb dakota.rst dakota.pdb"

Unrolls all data associated with a particular tag for all evaluations and then writes this data in a tabular format (e.g., to a PDB database or MATLAB/TECPLOT data file).

References abort_handler(), Variables::continuous_variables(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), and Response::function_values().

Referenced by main().

void print_restart_tabular ( StringArray pos_args, String print_dest, unsigned short tabular_format, int tabular_precision )

print a restart file (tabular format)

Usage: "dakota_restart_util to_tabular dakota.rst dakota.txt"

Unrolls all data associated with a particular tag for all evaluations and then writes this data in a tabular format (e.g., to a PDB database or MATLAB/TECPLOT data file).
References abort_handler(), Variables::acv(), Variables::adiv(), Variables::adrv(), Variables::adsv(), Variables::all_continuous_variable_labels(), Variables::all_discrete_int_variable_labels(), Variables::all_discrete_real_variable_labels(), Variables::all_discrete_string_variable_labels(), Response::function_labels(), ParamResponsePair::interface_id(), ParamResponsePair::response(), ParamResponsePair::variables(), write_precision, ParamResponsePair::write_tabular(), and ParamResponsePair::write_tabular_labels.

Referenced by main().

```cpp
void read_neutral ( StringArray pos_args )
```

read a restart file (neutral file format)

Usage: "dakota_restart_util from_neutral dakota.neu dakota.rst"

Reads evaluations from a neutral file. This is used for translating binary files between platforms.

References abort_handler(), and ParamResponsePair::read_annotated().

Referenced by main().

```cpp
void repair_restart ( StringArray pos_args, String identifier_type )
```

repair a restart file by removing corrupted evaluations

Usage: "dakota_restart_util remove 0.0 dakota_old.rst dakota_new.rst"
"dakota_restart_util remove_ids 2 7 13 dakota_old.rst dakota_new.rst"

Repairs a restart file by removing corrupted evaluations. The identifier for evaluation removal can be either a double precision number (all evaluations having a matching response function value are removed) or a list of integers (all evaluations with matching evaluation ids are removed).

References abort_handler(), Response::active_set_request_vector(), contains(), ParamResponsePair::eval_id(), Response::function_values(), and ParamResponsePair::response().

Referenced by main().

```cpp
void concatenate_restart ( StringArray pos_args )
```

concatenate multiple restart files

Usage: "dakota_restart_util cat dakota_1.rst ... dakota_n.rst dakota_new.rst"

Combines multiple restart files into a single restart database.

References abort_handler().

Referenced by main().

```cpp
std::vector<std::string> Dakota::get_pathext ( )
```

Utility function for executable file search algorithms

Referenced by WorkdirHelper::which().

```cpp
bool Dakota::contains ( const bfs::path & dir_path, const std::string & file_name, boost::filesystem::path & complete_filepath ) [inline]
```

Utility function for "which" sets complete_filepath from dir_path/file_name combo

### 12.1.5 Variable Documentation

```cpp
short abort_mode = ABORT_EXIT
```

by default Dakota exits or calls MPI_ABORT on errors
whether dakota exits/aborts or throws on errors
Referenced by `abort_throw_or_exit()`, `Environment::exit_mode()`, and `PythonInterface::python_run()`.

**Dakota_funcs DakFuncs0**

**Initial value:**

```c
= {
   fprintf,
   abort_handler,
   solver_option,
   continuous_lower_bounds1,
   continuous_upper_bounds1,
   nonlinear_ineq_constraints_lower_bounds1,
   nonlinear_ineq_constraints_upper_bounds1,
   nonlinear_eq_constraints_targets1,
   linear_ineq_constraints_lower_bounds1,
   linear_ineq_constraints_upper_bounds1,
   linear_eq_constraints_targets1,
   linear_eq_constraints_coeffs1,
   linear_eq_constraint_coeffs1,
   ComputeResponses1,
   GetFuncs1,
   GetGrads1,
   GetContVars1,
   SetBestContVars1,
   SetBestDiscVars1,
   SetBestRespFns1,
   Get_Real1,
   Get_Int1,
   Get_Bool1
}
```

**const char**\* FIELD_NAMES[ ]

**Initial value:**

```c
= { "numFns", "numVars", "numACV", "numADIV",
   "numADR", "numDerivVars", "x\text{C}", "x\text{D}",
   "x\text{R}", "x\text{Labels}", "x\text{DLabels}",
   "x\text{RLabels}", "directFnASV", "directFnDVV",
   "fnFlag", "gradFlag", "hessFlag",
   "fnVals", "fnGrads", "fnHessians",
   "fnLabels", "failure", "currEvalId" }
```

fields to pass to Matlab in Dakota structure

Referenced by `MatlabInterface::matlab_engine_run()`, and `MatlabInterface::MatlabInterface()`.

**const int NUMBER_OF_FIELDS = 23**

number of fields in above structure

Referenced by `MatlabInterface::matlab_engine_run()`, and `MatlabInterface::MatlabInterface()`.

**Var_uinfo CAUVLbl[CAUVar_Nkinds] [static]**

**Initial value:**

```c
= {
   VarLabelInfo(nuv_, NormalUnc),
   VarLabelInfo(lnuv_, LognormalUnc),
   VarLabelInfo(uuv_, UniformUnc),
   VarLabelInfo(luuv_, LoguniformUnc),
   VarLabelInfo(tuv_, TriangularUnc),
   VarLabelInfo(euv_, ExponentialUnc),
   VarLabelInfo(beuv_, BetaUnc),
```
VarLabelInfo(gauv_, GammaUnc),
VarLabelInfo(guuv_, GumbelUnc),
VarLabelInfo(fuv_, FrechetUnc),
VarLabelInfo(wuv_, WeibullUnc),
VarLabelInfo(hbuv_, HistogramBinUnc)
}

Var_uinfo DAUIVLbl[DAUIVar_Nkinds] [static]
Initial value:

= 
  VarLabelInfo(puv_, PoissonUnc),
  VarLabelInfo(biuv_, BinomialUnc),
  VarLabelInfo(nbuv_, NegBinomialUnc),
  VarLabelInfo(geuv_, GeometricUnc),
  VarLabelInfo(hguv_, HyperGeomUnc),
  VarLabelInfo(hpiuv_, HistogramPtIntUnc)
}

Var_uinfo DAUSVLbl[DAUSVar_Nkinds] [static]
Initial value:

= 
  VarLabelInfo(hpsuv_, HistogramPtStrUnc)

Var_uinfo DAURVLbl[DAURVar_Nkinds] [static]
Initial value:

= 
  VarLabelInfo(hpruv_, HistogramPtRealUnc)

Var_uinfo CEUVLbl[CEUVar_Nkinds] [static]
Initial value:

= 
  VarLabelInfo(ciuv_, ContinuousIntervalUnc)

Var_uinfo DEUIVLbl[DEUIVar_Nkinds] [static]
Initial value:

= 
  VarLabelInfo(diuv_, DiscreteIntervalUnc),
  VarLabelInfo(duisiv_, DiscreteUncSetInt)
12.1. DAKOTA NAMESPACE REFERENCE

Var_uinfo DEUSVLbl[DEUSVar_Nkinds] [static]
Initial value:

= {
  VarLabelInfo(dussv, DiscreteUncSetStr)
}

Var_uinfo DEURVLbl[DEURVar_Nkinds] [static]
Initial value:

= {
  VarLabelInfo(dusrv, DiscreteUncSetReal)
}

Var_uinfo DiscSetLbl[DiscSetVar_Nkinds] [static]
Initial value:

= {
  VarLabelInfo(ddsiv, DiscreteDesSetInt),
  VarLabelInfo(ddssv, DiscreteDesSetStr),
  VarLabelInfo(ddsrv, DiscreteDesSetReal),
  VarLabelInfo(ddssiv, DiscreteStateSetInt),
  VarLabelInfo(ddsssv, DiscreteStateSetStr),
  VarLabelInfo(ddssrv, DiscreteStateSetReal)
}

VarLabelChk DesignAndStateLabelsCheck[] [static]
Initial value:

= {
  {AVI numContinuousDesVars, AVI continuousDesignLabels, "cdv", "cdv.descriptors" },
  {AVI numDiscreteDesRangeVars, AVI discreteDesignRangeLabels, "ddriv", "ddriv.descriptors" },
  {AVI numDiscreteDesSetIntVars, AVI discreteDesignSetIntLabels, "ddsiv", "ddsiv.descriptors" },
  {AVI numDiscreteDesSetStrVars, AVI discreteDesignSetStrLabels, "ddssv", "ddssv.descriptors" },
  {AVI numDiscreteDesSetRealVars, AVI discreteDesignSetRealLabels, "ddsrv", "ddsrv.descriptors" },
  {AVI numContinuousStateVars, AVI continuousStateLabels, "csv", "csv.descriptors" },
  {AVI numDiscreteStateRangeVars, AVI discreteStateRangeLabels, "dssrv", "dssrv.descriptors" },
  {AVI numDiscreteStateSetIntVars, AVI discreteStateSetIntLabels, "dssiv", "dssiv.descriptors" },
  {AVI numDiscreteStateSetStrVars, AVI discreteStateSetStrLabels, "dsssv", "dsssv.descriptors" },
  {AVI numDiscreteStateSetRealVars, AVI discreteStateSetRealLabels, "dssrv", "dssrv.descriptors" },
  {AVI numContinuousDesVars, AVI continuousDesignScaleTypes, 0, "cdv.scale_types" }
}

Variables label array designations for design and state. All non-uncertain variables need to be in this array. Used in check_variables_node to check lengths and make_variable_defaults to build labels.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_defaults().

VLreal VLUncertainReal[NUM_UNC_REAL_CONT] [static]
Initial value:
Variables labels/bounds/values check array for real-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., CAUVLbl, with the contiguous container in which they are stored.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_defaults().

VLint VLUncertainInt[NUM_UNC_INT_CONT] [static]
Initial value:

= {
  {DAUIVarNkinds, AVI DAUv, DAUVLbl,
   DVR discreteIntAleatoryUncLabels,
   DVR discreteIntAleatoryUncLowerBnds,
   DVR discreteIntAleatoryUncUpperBnds,
   DVR discreteIntAleatoryUncVars},
  {DEUIVarNkinds, AVI DEUv, DEUVLbl,
   DVR discreteIntEpistemicUncLabels,
   DVR discreteIntEpistemicUncLowerBnds,
   DVR discreteIntEpistemicUncUpperBnds,
   DVR discreteIntEpistemicUncVars}}

Variables labels/bounds/values check array for integer-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUVLbl, with the contiguous container in which they are stored.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_defaults().

VLstr VLUncertainStr[NUM_UNC_STR_CONT] [static]
Initial value:

= {
  {DAUSVarNkinds, AVI DAUsv, DAUSLbl,
   DVR discreteStrAleatoryUncLabels,
   DVR discreteStrAleatoryUncLowerBnds,
   DVR discreteStrAleatoryUncUpperBnds,
   DVR discreteStrAleatoryUncVars},
  {DEUSVarNkinds, AVI DEUsv, DEUSLbl,
   DVR discreteStrEpistemicUncLabels,
   DVR discreteStrEpistemicUncLowerBnds,
   DVR discreteStrEpistemicUncUpperBnds,
   DVR discreteStrEpistemicUncVars}}
12.1. DAKOTA NAMESPACE REFERENCE

Variables labels/bounds/values check array for string-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUSVLbl, with the contiguous container in which they are stored.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_defaults().

Var_check var_mp_check_cv[] [static]

Initial value:

```c
= { 
  Vchk3(continuous_design,ContinuousDes), 
  Vchk3(continuous_state,ContinuousState) 
}
```

Var_check var_mp_check_dset[] [static]

Initial value:

```c
= { 
  Vchk3(discrete_design_set_integer,DiscreteDesSetInt), 
  Vchk3(discrete_design_set_string,DiscreteDesSetStr), 
  Vchk3(discrete_design_set_real,DiscreteDesSetReal), 
  Vchk3(discrete_state_set_integer,DiscreteStateSetInt), 
  Vchk3(discrete_state_set_string,DiscreteStateSetStr), 
  Vchk3(discrete_state_set_real,DiscreteStateSetReal) 
}
```

Var_check var_mp_check_cau[] [static]

Initial value:

```c
= { 
  Vchk3(normal_uncertain,NormalUnc), 
  Vchk3(lognormal_uncertain,LognormalUnc), 
  Vchk3(uniform_uncertain,UniformUnc), 
  Vchk3(loguniform_uncertain,LoguniformUnc), 
  Vchk3(triangular_uncertain,TriangularUnc), 
  Vchk3(exponential_uncertain,ExponentialUnc), 
  Vchk3(beta_uncertain,BetaUnc), 
  Vchk3(gamma_uncertain,GammaUnc), 
  Vchk3(gumbel_uncertain,GumbelUnc), 
  Vchk3(frechet_uncertain,FrechetUnc), 
  Vchk3(weibull_uncertain,WeibullUnc), 
  Vchk3(histogram_bin_uncertain,HistogramBinUnc) 
}
```

Var_check var_mp_check_daui[] [static]

Initial value:

```c
= { 
  Vchk3(poisson_uncertain,PoissonUnc), 
  Vchk3(binomial_uncertain,BinomialUnc), 
  Vchk3(negative_binomial_uncertain,NegBinomialUnc), 
  Vchk3(geometric_uncertain,GeometricUnc), 
  Vchk3(hypergeometric_uncertain,HyperGeomUnc), 
  Vchk3(histogram_point_int_uncertain,HistogramPtIntUnc) 
}
```
Var_check var_mp_check_daus[] [static]
Initial value:
= { 
    Vchk_3(histogram_point_str_uncertain,HistogramPtStrUnc) 
}

Var_check var_mp_check_daur[] [static]
Initial value:
= { 
    Vchk_3(histogram_point_real_uncertain,HistogramPtRealUnc) 
}

Var_check var_mp_check_ceu[] [static]
Initial value:
= { 
    Vchk_3(continuous_interval_uncertain,ContinuousIntervalUnc) 
}

Var_check var_mp_check_deui[] [static]
Initial value:
= { 
    Vchk_3(discrete_interval_uncertain,DiscreteIntervalUnc),
    Vchk_3(discrete_uncertain_set_integer,DiscreteUncSetInt) 
}

Var_check var_mp_check_deus[] [static]
Initial value:
= { 
    Vchk_3(discrete_uncertain_set_string,DiscreteUncSetStr) 
}

Var_check var_mp_check_deur[] [static]
Initial value:
= { 
    Vchk_3(discrete_uncertain_set_real,DiscreteUncSetReal) 
}
12.2 SIM NAMESPACE REFERENCE

**Var_rcheck var_mp_cbound[] [static]**

Initial value:

```cpp
= {
    Vchk,7(continuous_design, ContinuousDes, continuousDesign),
    Vchk,7(continuous_state, ContinuousState, continuousState),
    Vchk,5(normal_uncertain, NormalUnc, normalUnc),
    Vchk,5(lognormal_uncertain, LognormalUnc, lognormalUnc),
    Vchk,5(uniform_uncertain, UniformUnc, uniformUnc),
    Vchk,5(loguniform_uncertain, LoguniformUnc, loguniformUnc),
    Vchk,5(triangular_uncertain, TriangularUnc, triangularUnc),
    Vchk,5(beta_uncertain, BetaUnc, betaUnc) }
```

This is used within check_variables_node(): `Var_RealBoundIPCheck()` is applied to validate bounds and initial points.

Referenced by NIDRProblemDescDB::check_variables_node().

**Var_icheck var_mp_drange[] [static]**

Initial value:

```cpp
= {
    Vchk,7(discrete_design_range, DiscreteDesRange, discreteDesignRange),
    Vchk,7(discrete_state_range, DiscreteStateRange, discreteStateRange) }
```

This is used in check_variables_node(): `Var_IntBoundIPCheck()` is applied to validate bounds and initial points, and in make_variable_defaults(): `Vgen_*` is called to infer bounds.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_defaults().

**const char* SCI_FIELD_NAMES[]**

Initial value:

```cpp
= { "dakota_type", "numFns", "numVars", "numACV", "numADIV", "numADR", "numDerivVars", "xC", "xDI", "xDR", "xLabels", "xDILabels", "xDRLabels", "directFnASV", "directFnASM", "directFnDVV", "directFnDvVbool", "fnFlag", "gradFlag", "hessFlag", "fnVals", "fnGrads", "fnHessians", "fnLabels", "failure", "currEvalId" }
```

fields to pass to Scilab in Dakota structure

Referenced by ScilabInterface::scilab_engine_run().

**const int SCI_NUMBER_OF_FIELDS = 26**

number of fields in above structure

Referenced by ScilabInterface::scilab_engine_run().

12.2 SIM Namespace Reference

A sample namespace for derived classes that use assign_rep() to plug facilities into DAKOTA.
Classes

- class ParallelDirectApplicInterface
  
  *Sample derived interface class for testing parallel simulator plug-ins using assign_rep().*

- class SerialDirectApplicInterface
  
  *Sample derived interface class for testing serial simulator plug-ins using assign_rep().*

### 12.2.1 Detailed Description

A sample namespace for derived classes that use assign_rep() to plug facilities into DAKOTA. A typical use of plug-ins with assign_rep() is to publish a simulation interface for use in library mode. See [Interfacing with Dakota as a Library](#) for more information.
Chapter 13

Class Documentation

13.1 ActiveSet Class Reference

Container class for active set tracking information. Contains the active set request vector and the derivative variables vector.

Public Member Functions

- **ActiveSet ()**
  default constructor
- **ActiveSet (size_t num_fns, size_t num_deriv_vars)**
  standard constructor
- **ActiveSet (size_t num_fns)**
  partial constructor
- **ActiveSet (const ShortArray &asv, const SizetArray &dvv)**
  alt constructor
- **ActiveSet (const ActiveSet &set)**
  copy constructor
- **~ActiveSet ()**
  destructor
- **ActiveSet & operator= (const ActiveSet &set)**
  assignment operator
- **void reshape (size_t num_fns, size_t num_deriv_vars)**
  reshape requestVector and derivVarsVector
- **void reshape (size_t num_fns)**
  reshape requestVector
- **const ShortArray & request_vector () const**
  return the request vector
- **void request_vector (const ShortArray &rv)**
  set the request vector
- **void request_values (const short rv_val)**
  set all request vector values
• short request_value (const size_t index) const
  get the value of an entry in the request vector
• void request_value (const short rv_val, const size_t index)
  set the value of an entry in the request vector
• const SizetArray & derivative_vector () const
  return the derivative variables vector
• void derivative_vector (const SizetArray &dvv)
  set the derivative variables vector from a SizetArray
• void derivative_vector (SizetMultiArrayConstView dvv)
  set the derivative variables vector from a SizetMultiArrayConstView
• void derivative_start_value (size_t dvv_start_val)
  set the derivative variables vector values
• void read (std::istream &s)
  read an active set object from an std::istream
• void write (std::ostream &s) const
  write an active set object to an std::ostream
• void write.annotated (std::ostream &s) const
  write an active set object to an std::ostream in annotated format
• void read (MPIUnpackBuffer &s)
  read an active set object from a packed MPI buffer
• void write (MPIPackBuffer &s) const
  write an active set object to a packed MPI buffer

Private Member Functions

• template<class Archive>
  void serialize (Archive &ar, const unsigned int version)
  implementation of Boost serialize for ActiveSet

Private Attributes

• ShortArray requestVector
  the vector of response requests
• SizetArray derivVarsVector
  the vector of variable ids used for computing derivatives

Friends

• class boost::serialization::access
• bool operator== (const ActiveSet &set1, const ActiveSet &set2)
  equality operator
• bool operator!= (const ActiveSet &set1, const ActiveSet &set2)
  inequality operator
13.2. ACTIVESUBSPACEMODEL CLASS REFERENCE

13.1.1 Detailed Description

Container class for active set tracking information. Contains the active set request vector and the derivative variables vector.

The ActiveSet class is a small class whose initial design function is to avoid having to pass the ASV and DVV separately. It is not part of a class hierarchy and does not employ reference-counting/representation-sharing idioms (e.g., handle-body).

13.1.2 Member Data Documentation

ShortArray requestVector [private]
the vector of response requests

It uses a 0 value for inactive functions and sums 1 (value), 2 (gradient), and 4 (Hessian) for active functions.

Referenced by ActiveSet::ActiveSet(), ActiveSet::operator=(), ActiveSet::read(), ActiveSet::request_value(), ActiveSet::request_values(), ActiveSet::request_vector(), ActiveSet::reshape(), ActiveSet::write(), and ActiveSet::write_annotated().

SizetArray derivVarsVector [private]
the vector of variable ids used for computing derivatives

These ids will generally identify either the active continuous variables or the inactive continuous variables.

Referenced by ActiveSet::ActiveSet(), ActiveSet::derivative_start_value(), ActiveSet::derivative_vector(), ActiveSet::operator=(), ActiveSet::read(), ActiveSet::reshape(), ActiveSet::write(), and ActiveSet::write_annotated().

The documentation for this class was generated from the following file:

- DakotaActiveSet.hpp

13.2 ActiveSubspaceModel Class Reference

Active subspace model for input (variable space) reduction.

Inheritance diagram for ActiveSubspaceModel:

```
Model
   |
   +---- RecastModel
       |
       +---- ActiveSubspaceModel
```

Public Member Functions

- ActiveSubspaceModel (ProblemDescDB &problem_db)
  
  *Problem database constructor.*

- ActiveSubspaceModel (const Model &sub_model, unsigned int dimension, const RealMatrix &rotation_matrix, short output_level)
  
  *Lightweight constructor*

- ~ActiveSubspaceModel ()
### Destructor

- `bool initialize_mapping (ParLevLIter pl_iter)`
- `bool finalize_mapping ()`
  - finalize model mapping, returns true if the variables size has changed
- `bool mapping_initialized () const`
  - return true if mapping has been fully initialized, false otherwise.
- `bool resize_pending () const`
  - return true if a potential resize is still pending, such that sizing-based initialization should be deferred
- `void stop_init_mapping (ParLevLIter pl_iter)`
  - called from `IteratorScheduler::init_iterator()` for iteratorComm rank 0 to terminate `serve_init_mapping()` on other iteratorComm processors
- `int serve_init_mapping (ParLevLIter pl_iter)`
  - called from `IteratorScheduler::init_iterator()` for iteratorComm rank != 0 to balance resize() calls on iteratorComm rank 0

### Protected Member Functions

- `void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)`
- `void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)`
  - portion of `set_communicators()` specific to derived model classes
- `void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)`
  - portion of `free_communicators()` specific to derived model classes
- `void derived_evaluate (const ActiveSet &set)`
  - portion of `evaluate()` specific to derived model classes
- `void derived_evaluate_nowait (const ActiveSet &set)`
  - portion of `evaluate_nowait()` specific to derived model classes
- `const IntResponseMap & derived_synchronize ()`
  - portion of `synchronize()` specific to derived model classes
- `const IntResponseMap & derived_synchronize_nowait ()`
  - portion of `synchronize_nowait()` specific to derived model classes
- `void component_parallel_mode (short mode)`
  - update component parallel mode for supporting parallelism in the offline and online phases
- `void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)`
  - Service the offline and online phase job requests received from the master; completes when termination message received from `stop_servers()`.
- `void stop_servers ()`
  - Executed by the master to terminate the offline and online phase server operations when iteration on the `ActiveSubspaceModel` is complete.
- `Model get_sub_model (ProblemDescDB &problem_db)`
  - retrieve the sub-Model from the DB to pass up the constructor chain
- `void init_fullspace_sampler (unsigned short sample_type)`
  - initialize the native problem space Monte Carlo sampler
- `void validate_inputs ()`
  - validate the build controls and set defaults
• void build_subspace ()
  sample the model’s gradient, computed the SVD, and form the active subspace rotation matrix.

• void generate_fullspace_samples (unsigned int diff_samples)
  sample the derivative at diff_samples points and leave temporary in dace_iterator

• void populate_matrices (unsigned int diff_samples)
  populate the derivative and vars matrices with fullSpaceSampler samples

• void compute_svd ()
  factor the derivative matrix and analyze singular values, assessing convergence and rank, returning whether tolerance met

• void identify_subspace ()
  use the truncation methods to identify the size of an active subspace

• unsigned int computeBingLiCriterion (RealVector &singular_values)
  compute Bing Li’s criterion to identify the active subspace

• unsigned int computeConstantineMetric (RealVector &singular_values)
  compute Constantine’s metric to identify the active subspace

• unsigned int computeEnergyCriterion (RealVector &singular_values)
  Compute active subspace size based on eigenvalue energy. Compatible with other truncation methods.

• unsigned int computeCrossValidationMetric ()
  Use cross validation of a moving least squares surrogate to identify the size of an active subspace that meets an error tolerance.

• Real build_cv_surrogate (Model &cv_surr_model, RealMatrix training_x, IntResponseMap training_y, RealMatrix test_x, IntResponseMap test_y)
  Build moving least squares surrogate over candidate active subspace.

• unsigned int determine_rank_cv (const std::vector< Real > &cv_error)

• unsigned int min_index (const std::vector< Real > &cv_error)

• unsigned int tolerance_met_index (const std::vector< Real > &cv_error, Real tolerance, bool &tol_met)

• std::vector< Real > negative_diff (const std::vector< Real > &cv_error)

• void build_surrogate ()
  Build surrogate over active subspace.

• void initialize_recast ()
  Initialize the base class RecastModel with reduced space variable sizes.

• SizetArray variables_resize ()
  Create a variables components totals array with the reduced space size for continuous variables.

• void uncertain_vars_to_subspace ()
  translate the characterization of uncertain variables in the native model to the reduced space of the transformed model

• void update_linear_constraints ()
  transform the original bounded domain (and any existing linear constraints) into linear constraints in the reduced space

• void update_var_labels ()
  update variable labels
Static Protected Member Functions

- static void `vars_mapping` (const `Variables` &recast_xi_vars, `Variables` &sub_model_x_vars)
  map the active continuous recast variables to the active submodel variables (linear transformation)
- static void `set_mapping` (const `Variables` &recast_vars, const `ActiveSet` &recast_set, `ActiveSet` &sub_model_set)
  map the inbound `ActiveSet` to the sub-model (map derivative variables)
- static void `response_mapping` (const `Variables` &recast_y_vars, const `Variables` &sub_model_x_vars, const `Response` &sub_model_resp, `Response` &recast_resp)
  map responses from the sub-model to the recast model

Protected Attributes

- int `randomSeed`
  seed controlling all samplers
- int `initialSamples`
  initial number of samples at which to query the truth model
- int `maxFunctionEvals`
  maximum number of build evaluations
- bool `subspaceIdBingLi`
  Boolean flag signaling use of Bing Li criterion to identify active subspace dimension.
- bool `subspaceIdConstantine`
  Boolean flag signaling use of Constantine criterion to identify active subspace dimension.
- bool `subspaceIdEnergy`
  Boolean flag signaling use of eigenvalue energy criterion to identify active subspace dimension.
- bool `subspaceIdCV`
  Boolean flag signaling use of cross validation to identify active subspace dimension.
- size_t `numReplicates`
  Number of bootstrap samples for subspace identification.
- bool `transformVars`
  boolean flag to determine if variables should be transformed to u-space before active subspace initialization
- size_t `numFullspaceVars`
  Number of fullspace active continuous variables.
- size_t `numFunctions`
  Total number of response functions.
- unsigned int `totalSamples`
  total construction samples evaluated so far
- bool `subspaceInitialized`
  boolean flag to determine if mapping has been fully initialized
- unsigned short `subspaceNormalization`
  Normalization to use in the case of multiple QoI’s.
- unsigned int `reducedRank`
  current approximation of system rank
- RealMatrix `activeBasis`
13.2. ACTIVESUBSPACEMODEL CLASS REFERENCE

- **RealMatrix inactiveBasis**
  basis for the inactive subspace
- **RealVector inactiveVars**
  current inactive variables
- **RealMatrix derivativeMatrix**
  matrix of derivative data with numFunctions columns per fullspace sample; each column contains the gradient of one function at one sample point, so total matrix size is numContinuousVars * (numFunctions * numSamples) [D1 | D2 | ... | Dnum_samples] [dy1/dx(k=1) | dy2/dx(k=1) | ... | dyM/dx(k=1) | k=2 | ... | k=n_s]
- **RealMatrix leftSingularVectors**
  matrix of the left singular vectors of derivativeMatrix
- **RealVector singularValues**
  singular values of derivativeMatrix
- **RealMatrix varsMatrix**
  matrix of fullspace variable points samples size numContinuousVars * (numSamples)
- **RealArray gradientScaleFactors**
  Gradient scaling factors to make multiple response function gradients similar orders of magnitude.
- **Real truncationTolerance**
  Truncation tolerance for eigenvalue energy subspace identification.
- **bool cvIncremental**
- **short cvIdMethod**
- **Real cvRefTolerance**
- **Real cvDecreaseTolerance**
- **unsigned int cvMaxRank**
  maximum subspace size to consider using cross validation
- **Model surrogateModel**
  model containing a surrogate built over the active subspace
- **bool buildSurrogate**
  flag specifying whether or not a surrogate is built over the subspace
- **int refinementSamples**
  Number of refinement samples to use when building a surrogate.
- **Iterator fullspaceSampler**
  Monte Carlo sampler for the full parameter space.
- **size_t miPLIndex**
  the index of the active metaiterator-iterator parallelism level (corresponding to ParallelConfiguration::miPLIters) used at runtime
- **int onlineEvalConcurrency**
  Concurrency to use once subspace has been built.
- **int offlineEvalConcurrency**
  Concurrency to use when building subspace.
- **IntResponseMap surrResponseMap**
  map of responses returned in buildSurrogate mode
- **IntIntMap surrIdMap**
  map from surrogateModel evaluation ids to RecastModel ids
Static Protected Attributes

- static ActiveSubspaceModel * asmInstance
  
  static pointer to this class for use in static callbacks

Additional Inherited Members

13.2.1 Detailed Description

Active subspace model for input (variable space) reduction.
Specialization of a RecastModel that identifies an active subspace during build phase and creates a RecastModel in the reduced space

13.2.2 Constructor & Destructor Documentation

ActiveSubspaceModel ( const Model & sub_model, unsigned int dimension, const RealMatrix & rotation_matrix, short output_level )

lightweight constructor

An ActiveSubspaceModel will be built over all functions, without differentiating primary vs. secondary constraints. However the associated RecastModel has to differentiate. Currently identifies subspace for continuous variables only, but carries other active variables along for the ride.

References ActiveSubspaceModel::activeBasis, ActiveSubspaceModel::build_surrogate(), ActiveSubspaceModel::buildSurrogate, Model::componentParallelMode, Model::derivative_concurrency(), ActiveSubspaceModel::inactive-Basis, ActiveSubspaceModel::initialize_recast(), ActiveSubspaceModel::initialSamples, Model::modelType, ActiveSubspaceModel::numFullspaceVars, ActiveSubspaceModel::offlineEvalConcurrency, ActiveSubspaceModel::onlineEvalConcurrency, Model::output_level(), Model::outputLevel, ActiveSubspaceModel::reducedRank, RecastModel::subModel, ActiveSubspaceModel::subspaceInitialized, Model::supportsEstimDerivs, ActiveSubspaceModel::uncertain_vars_to_subspace(), ActiveSubspaceModel::update_linear_constraints(), and ActiveSubspaceModel::update_var_labels().

13.2.3 Member Function Documentation

bool initialize_mapping ( ParLevLIter pl_iter ) [virtual]

May eventually take on init_comms and related operations. Also may want ide of build/update like DataFitSurr-Model, eventually.

Reimplemented from Model.

References ActiveSubspaceModel::build_subspace(), ActiveSubspaceModel::build_surrogate(), ActiveSubspaceModel::buildSurrogate, ActiveSubspaceModel::component_parallel_mode(), Model::initialize_mapping(), RecastModel::initialize_mapping(), ActiveSubspaceModel::initialize_recast(), ActiveSubspaceModel::miPLIndex, Model::modelPCIter, ActiveSubspaceModel::numFullspaceVars, Model::outputLevel, ActiveSubspaceModel::reducedRank, RecastModel::subModel, ActiveSubspaceModel::subspaceInitialized, Model::supportsEstimDerivs, ActiveSubspaceModel::uncertain_vars_to_subspace(), ActiveSubspaceModel::update_linear_constraints(), and ActiveSubspaceModel::update_var_labels().

void derived_init_communicators ( ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag ) [protected], [virtual]

This specialization is because the model is used in multiple contexts in this iterator, depending on build phase. Note that this overrides the default behavior at Iterator which recurses into any submodels.
13.2. ACTIVESUBSPACEMODEL CLASS REFERENCE

Reimplemented from Model.
References ActiveSubspaceModel::fullspaceSampler, Iterator::init_communicators(), Model::init_communicators(), ActiveSubspaceModel::onlineEvalConcurrency, RecastModel::subModel, and ActiveSubspaceModel::subspaceInitialized.

**Real build_cv.surrogate ( Model & cv.surr_model, RealMatrix training_x, IntResponseMap training_y, RealMatrix test_x, IntResponseMap test_y ) [protected]**

Build moving least squares surrogate over candidate active subspace.
- Build global moving least squares surrogate model to use in cross validation to estimate active subspace size.
  References Response::active_set(), Model::continuous_variables(), Response::copy(), Model::current_response(), Model::evaluate(), ActiveSubspaceModel::numFunctions, and Model::update_approximation.
  Referenced by ActiveSubspaceModel::computeCrossValidationMetric().

**void build_surrogate ( ) [protected]**

Build surrogate over active subspace.
- Build surrogate over active subspace
  References Response::active_set(), Iterator::active_set(), ActiveSubspaceModel::activeBasis, Iterator::all_responses(), Iterator::all_samples(), Model::append_approximation(), ActiveSubspaceModel::asmInstance, Model::assign_rep(), Model::current_response(), ActiveSubspaceModel::fullspaceSampler, ActiveSubspaceModel::miPLIndex, Model::modelPCIter, Model::outputLevel, ActiveSubspaceModel::reducedRank, ActiveSubspaceModel::refinementSamples, ActiveSet::request_values(), Iterator::run(), Iterator::sampling_reference(), Iterator::sampling_reset(), and ActiveSubspaceModel::surrogateModel.
  Referenced by ActiveSubspaceModel::ActiveSubspaceModel(), and ActiveSubspaceModel::initialize_mapping().

**void initialize_recast ( ) [protected]**

Initialize the base class RecastModel with reduced space variable sizes.
- Initialize the recast model based on the reduced space, with no response function mapping (for now). TODO: use a surrogate model over the inactive dimension.
  References Model::current_response(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), Response::function_gradients(), Response::function_hessians(), RecastModel::init_maps(), RecastModel::init_sizes(), Model::num_functions(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), ActiveSubspaceModel::numFunctions, ActiveSubspaceModel::reducedRank, ActiveSubspaceModel::response_mapping(), ActiveSubspaceModel::set_mapping(), RecastModel::subModel, ActiveSubspaceModel::variables_resize(), and ActiveSubspaceModel::vars_mapping().
  Referenced by ActiveSubspaceModel::ActiveSubspaceModel(), and ActiveSubspaceModel::initialize_mapping().

**void uncertain_vars_to_subspace ( ) [protected]**

translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model
- transform and set the distribution parameters in the reduced model
  Convert the user-specified normal random variables to the appropriate reduced space variables, based on the orthogonal transformation.
  TODO: Generalize to convert other random variable types (non-normal)
  TODO: The translation of the correlations from full to reduced space is likely wrong for rank correlations; should be correct for covariance.
  Referenced by ActiveSubspaceModel::ActiveSubspaceModel(), and ActiveSubspaceModel::initialize_mapping().
void vars_mapping ( const Variables & recast_y_vars, Variables & sub_model_x_vars ) [static], [protected]

map the active continuous recast variables to the active submodel variables (linear transformation)

Perform the variables mapping from recast reduced dimension variables y to original model x variables via linear transformation. Maps only continuous variables.

References ActiveSubspaceModel::activeBasis, ActiveSubspaceModel::asmInstance, Variables::continuous_variables(), Dakota::copy_data(), ActiveSubspaceModel::inactiveBasis, ActiveSubspaceModel::inactiveVars, and Model::outputLevel.

Referenced by ActiveSubspaceModel::initialize_recast().

void set_mapping ( const Variables & recast_vars, const ActiveSet & recast_set, ActiveSet & sub_model_set ) [static], [protected]

map the inbound ActiveSet to the sub-model (map derivative variables)

Simplified derivative variables mapping where all continuous depend on all others. TODO: Could instead rely on a richer default in RecastModel based on varsMapIndices.

References ActiveSubspaceModel::asmInstance, Variables::cv(), Model::cv(), ActiveSet::derivative_vector(), and RecastModel::subModel.

Referenced by ActiveSubspaceModel::initialize_recast().

void response_mapping ( const Variables & recast_y_vars, const Variables & sub_model_x_vars, const Response & sub_modelResp, Response & recastResp ) [static], [protected]

map responses from the sub-model to the recast model

Perform the response mapping from submodel to recast response

References ActiveSubspaceModel::activeBasis, ActiveSubspaceModel::asmInstance, Response::function_gradients(), Response::function_hessians(), and Response::function_values().

Referenced by ActiveSubspaceModel::initialize_recast().

13.2.4 Member Data Documentation

ActiveSubspaceModel * asmInstance [static], [protected]

static pointer to this class for use in static callbacks

initialization of static needed by RecastModel

Referenced by ActiveSubspaceModel::ActiveSubspaceModel(), ActiveSubspaceModel::build_surrogate(), ActiveSubspaceModel::response_mapping(), ActiveSubspaceModel::set_mapping(), and ActiveSubspaceModel::vars_mapping().

The documentation for this class was generated from the following files:

- ActiveSubspaceModel.hpp
- ActiveSubspaceModel.cpp

13.3 AdaptedBasisModel Class Reference

Adapted basis model for input (variable space) reduction.

Inheritance diagram for AdaptedBasisModel:
13.3. ADAPTEDBASISMODEL CLASS REFERENCE

Public Member Functions

- AdaptedBasisModel (ProblemDescDB &problem_db)
  Problem database constructor.
- ~AdaptedBasisModel ()
  Destructor.
- bool initialize_mapping (ParLevLIter pl_iter)
  Initialize model mapping, returns true if the variables size has changed.
- bool finalize_mapping ()
  Finalize model mapping, returns true if the variables size has changed.
- bool mapping_initialized () const
  Return true if mapping has been fully initialized, false otherwise.
- bool resize_pending () const
  Return true if a potential resize is still pending, such that sizing-based initialization should be deferred.
- void stop_init_mapping (ParLevLIter pl_iter)
  Called from IteratorScheduler::init_iterator() for iteratorComm rank 0 to terminate serve_init_mapping() on other iteratorComm processors.
- int serve_init_mapping (ParLevLIter pl_iter)
  Called from IteratorScheduler::init_iterator() for iteratorComm rank != 0 to balance resize() calls on iteratorComm rank 0.

Protected Member Functions

- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)
  Portion of set_communicators() specific to derived model classes.
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)
  Portion of free_communicators() specific to derived model classes.
- void derived_evaluate (const ActiveSet &set)
  Portion of evaluate() specific to derived model classes.
- void derived_evaluate_nowait (const ActiveSet &set)
  Portion of evaluate_nowait() specific to derived model classes.
- const IntResponseMap & derived_synchronize ()
  Portion of synchronize() specific to derived model classes.
- const IntResponseMap & derived_synchronize_nowait ()
  Portion of synchronize_nowait() specific to derived model classes.
• void component\_parallel\_mode (short mode)
  
  update component parallel mode for supporting parallelism in the offline and online phases

• void serve\_run (ParLevLIter pl\_iter, int max\_eval\_concurrency)
  
  Service the offline and online phase job requests received from the master; completes when termination message received from stop\_server().

• void stop\_servers ()
  
  Executed by the master to terminate the offline and online phase server operations when iteration on the Adapted-BasisModel is complete.

• Model get\_sub\_model (ProblemDescDB &problem\_db)
  
  retrieve the sub-Model from the DB to pass up the constructor chain

• void validate\_inputs ()
  
  validate the build controls and set defaults

• void identify\_subspace ()

• void initialize\_recast ()
  
  Initialize the base class RecastModel with reduced space variable sizes.

• SizetArray variables\_resize ()
  
  Create a variables components totals array with the reduced space size for continuous variables.

• void uncertain\_vars\_to\_subspace ()
  
  translate the characterization of uncertain variables in the native model to the reduced space of the transformed model

Static Protected Member Functions

• static void vars\_mapping (const Variables &recast\_xi\_vars, Variables &sub\_model\_x\_vars)
  
  map the active continuous recast variables to the active submodel variables (linear transformation)

• static void set\_mapping (const Variables &recast\_vars, const ActiveSet &recast\_set, ActiveSet &sub\_model\_set)
  
  map the inbound ActiveSet to the sub-model (map derivative variables)

• static void response\_mapping (const Variables &recast\_y\_vars, const Variables &sub\_model\_x\_vars, const Response &sub\_model\_resp, Response &recast\_resp)
  
  map responses from the sub-model to the recast model

Protected Attributes

• Iterator * pcePilotExpRepPtr
  
  PCE representation pointer that is initialized in get\_sub\_model() and then assigned into pcePilotExpansion in the constructor initializer list.

• Iterator pcePilotExpansion
  
  low-order (linear or quadratic) PCE generator for computing rotation matrices $A_j$ for each of the QoI; this is low-order and potentially high-dimension whereas a client PCE could be high-order in the reduced dimension

• size\_t numFullspaceVars
  
  Number of fullspace active continuous variables.

• size\_t numFunctions
  
  Total number of response functions.

• bool adaptedBasisInitialized
boolean flag to determine if mapping has been fully initialized

- unsigned int reducedRank
  current approximation of system rank
- RealMatrix rotationMatrix
  basis for the reduced subspace
- size_t miPLIndex
  the index of the active metaiterator-iterator parallelism level (corresponding to ParallelConfiguration::miPLIters) used at runtime
- int onlineEvalConcurrency
  Concurrency to use once subspace has been built.
- int offlineEvalConcurrency
  Concurrency to use when building subspace.

Static Protected Attributes

- static AdaptedBasisModel * abmInstance
  static pointer to this class for use in static callbacks

Additional Inherited Members

13.3.1 Detailed Description

Adapted basis model for input (variable space) reduction. Specialization of a RecastModel that creates an adapted basis model during build phase and creates a RecastModel in the reduced space

13.3.2 Member Function Documentation

void derived_init_communicators ( ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag )
[inline], [protected], [virtual]

This specialization is because the model is used in multiple contexts depending on build phase. Reimplemented from Model.

References Iterator::init_communicators(), Model::init_communicators(), AdaptedBasisModel::onlineEvalConcurrency, AdaptedBasisModel::pcePilotExpansion, and RecastModel::subModel.

void initialize_recast ( ) [protected]

Initialize the base class RecastModel with reduced space variable sizes.

Initialize the recast model based on the reduced space, with no response function mapping (for now).

References Model::current_response(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), Response::function_gradients(), Response::function_hessians(), RecastModel::init_maps(), RecastModel::init_sizes(), Model::num_functions(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), AdaptedBasisModel::reducedRank, AdaptedBasisModel::response_mapping(), AdaptedBasisModel::set_mapping(), RecastModel::subModel, AdaptedBasisModel::variables_resize(), and AdaptedBasisModel::vars_mapping.

Referenced by AdaptedBasisModel::initialize_mapping().
void uncertain_vars_to_subspace() [protected]
translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model
   transform and set the distribution parameters in the reduced model
   Convert the user-specified normal random variables to the appropriate reduced space variables, based on the orthogonal transformation.
   TODO: Generalize to convert other random variable types (non-normal)
   TODO: The translation of the correlations from full to reduced space is likely wrong for rank correlations; should be correct for covariance.
   Referenced by AdaptedBasisModel::initialize_mapping().

void vars_mapping (const Variables &recast_y_vars, Variables &sub_model_x_vars) [static], [protected]
map the active continuous recast variables to the active submodel variables (linear transformation)
   Perform the variables mapping from recast reduced dimension variables y to original model x variables via linear transformation. Maps only continuous variables.
   References AdaptedBasisModel::abmInstance, Variables::continuous_variables(), Variables::continuous_variables_view(), Model::outputLevel, and AdaptedBasisModel::rotationMatrix.
   Referenced by AdaptedBasisModel::initialize_recast().

void set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set) [static], [protected]
map the inbound ActiveSet to the sub-model (map derivative variables)
   Simplified derivative variables mapping where all continuous depend on all others. TODO: Could instead rely on a richer default in RecastModel based on varsMapIndices.
   References AdaptedBasisModel::abmInstance, Variables::cv(), Model::cv(), ActiveSet::derivative_vector(), and RecastModel::subModel.
   Referenced by AdaptedBasisModel::initialize_recast().

void response_mapping (const Variables &recast_y_vars, const Variables &sub_model_x_vars, const Response &sub_model_resp, Response &recast_resp) [static], [protected]
map responses from the sub-model to the recast model
   Perform the response mapping from submodel to recast response
   References AdaptedBasisModel::abmInstance, Response::function_gradients(), Response::function_hessians(), Response::function_values(), and AdaptedBasisModel::rotationMatrix.
   Referenced by AdaptedBasisModel::initialize_recast().

13.3.3 Member Data Documentation

AdaptedBasisModel *abmInstance [static], [protected]
static pointer to this class for use in static callbacks
   initialization of static needed by RecastModel
   Referenced by AdaptedBasisModel::AdaptedBasisModel(), AdaptedBasisModel::response_mapping(), AdaptedBasisModel::set_mapping(), and AdaptedBasisModel::vars_mapping().

The documentation for this class was generated from the following files:
13.4 Analyzer Class Reference

Base class for NonD, DACE, and ParamStudy branches of the iterator hierarchy.

Inheritance diagram for Analyzer:

```
Analyzer
  Iterator
    NonD
      NonDCalibration
      NonDExpansion
      NonDIntegration
      NonDInterval
      NonDPOFDarts
      NonDReliability
      NonDSampling
    PStudyDACE
      DDACEDesignCompExp
      FSUDesignCompExp
    Verification
      RichExtrapVerification
      ParamStudy
      PSUADERDesignCompExp
```

### Public Member Functions

- `const VariablesArray & all_variables ()`
  
  return the complete set of evaluated variables

- `const RealMatrix & all_samples ()`
  
  return the complete set of evaluated samples

- `const IntResponseMap & all_responses () const`
  
  return the complete set of computed responses

- `bool resize ()`
  
  reinitializes iterator based on new variable size

- `int num_samples () const`

- `virtual void vary_pattern (bool pattern_flag)`
  
  sets varyPattern in derived classes that support it

### Protected Member Functions

- `Analyzer ()`
  
  default constructor

- `Analyzer (ProblemDescDB &problem_db, Model &model)`
CHAPTER 13. CLASS DOCUMENTATION

- **Analyzer** (unsigned short method_name, Model &model)
  alternate constructor for instantiations "on the fly" with a Model

- **Analyzer** (unsigned short method_name)
  alternate constructor for instantiations "on the fly" without a Model

- \(~\text{Analyzer}()\)
  destructor

- virtual void get parameter sets (Model &model)
  Generate one block of numSamples samples (ndim \( \times \) num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.

- virtual void get parameter sets (Model &model, const int num_samples, RealMatrix &design_matrix)
  Generate one block of numSamples samples (ndim \( \times \) num_samples), populating design_matrix.

- virtual void update model from sample (Model &model, const Real∗ sample_vars)
  update model's current variables with data from sample

- virtual void update model from variables (Model &model, const Variables &vars)
  update model's current variables with data from vars

- virtual void sample to variables (const Real∗ sample_vars, Variables &vars)
  convert column of samples array to variables; derived classes may reimplement for more than active continuous variables

- void update from model (const Model &model)
  set inherited data attributes based on extractions from incoming model

- void initialize run ()
  utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

- void pre_run ()
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

- void post_run (std::ostream &s)
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

- void finalize run ()
  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

- void pre_output ()

- void print results (std::ostream &s)
  print the final iterator results

- const Model & algorithm space model () const

- const Variables & variables results () const
  return a single final iterator solution (variables)

- const Response & response results () const
  return a single final iterator solution (response)

- const VariablesArray & variables array results ()
  return multiple final iterator solutions (variables). This should only be used if returns multiple points() returns true.

- const ResponseArray & response array results ()
13.4. ANALYZER CLASS REFERENCE

return multiple final iterator solutions (response). This should only be used if `returns_multiple_points()` returns true.

- **void response_results_active_set (const ActiveSet &set)**  
  set the requested data for the final iterator response results

- **bool compact_mode () const**  
  returns Analyzer::compactMode

- **bool returns_multiple_points () const**  
  indicates if this iterator returns multiple final points. Default return is false. Override to return true if appropriate.

- **void evaluate_parameter_sets (Model &model, bool log.resp_flag, bool log.best_flag)**  
  perform function evaluations to map parameter sets (allVariables) into response sets (allResponses)

- **void get_vbd_parameter_sets (Model &model, int num_samples)**  
  generate replicate parameter sets for use in variance-based decomposition

- **void compute_vbd_stats (const int num_samples, const IntResponseMap &resp_samples)**  
  compute VBD-based Sobol indices

- **void read_variables_responses (int num_evals, size_t num_vars)**  
  convenience function for reading variables/responses (used in derived classes post_input)

- **void print_sobol_indices (std::ostream &s) const**  
  Printing of VBD results.

- **void samples_to_variables_array (const RealMatrix &sample_matrix, VariablesArray &vars_array)**  
  convert samples array to variables array; e.g., allSamples to allVariables

- **virtual void variables_to_sample (const Variables &vars, Real *sample_c(vars)**  
  convert the active continuous variables into a column of allSamples

- **void variables_array_to_samples (const VariablesArray &vars_array, RealMatrix &sample_matrix)**  
  convert variables array to samples array; e.g., allVariables to allSamples

**Protected Attributes**

- **size_t numFunctions**  
  number of response functions

- **size_t numContinuousVars**  
  number of active continuous vars

- **size_t numDiscreteIntVars**  
  number of active discrete integer vars

- **size_t numDiscreteStringVars**  
  number of active discrete string vars

- **size_t numDiscreteRealVars**  
  number of active discrete real vars

- **bool compactMode**  
  switch for allSamples (compact mode) instead of allVariables (normal mode)

- **VariablesArray allVariables**  
  array of all variables to be evaluated in `evaluate_parameter_sets()`

- **RealMatrix allSamples**  
  compact alternative to allVariables

- **IntResponseMap allResponses**
array of all responses to be computed in `evaluate_parameter_sets()`

- `StringArray allHeaders`
  array of headers to insert into output while evaluating `allVariables`

- `size_t numObjFns`
  number of objective functions

- `size_t numLsqTerms`
  number of least squares terms

- `RealPairPRPMultiMap bestVarsRespMap`
  map which stores best set of solutions

**Private Member Functions**

- `void compute_best_metrics (const Response &response, std::pair<Real, Real> &metrics)`
  compares current evaluation to best evaluation and updates best

- `void update_best (const Variables &vars, int eval_id, const Response &response)`
  compares current evaluation to best evaluation and updates best

- `void update_best (const Real *sample_c_vars, int eval_id, const Response &response)`
  compares current evaluation to best evaluation and updates best

**Private Attributes**

- `int writePrecision`
  write precision as specified by the user

- `Real vbdDropTol`
  tolerance for omitting output of small VBD indices

- `RealVectorArray S4`
  VBD main effect indices.

- `RealVectorArray T4`
  VBD total effect indices.

**Additional Inherited Members**

**13.4.1 Detailed Description**

Base class for `NonD`, DACE, and ParamStudy branches of the iterator hierarchy.

The Analyzer class provides common data and functionality for various types of systems analysis, including nondeterministic analysis, design of experiments, and parameter studies.

**13.4.2 Member Function Documentation**

`int num_samples () const [inline], [virtual]`

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from `Iterator`.

Reimplemented in `NonDSampling`, `NonDQuadrature`, `NonDSparseGrid`, `NonDCubature`, `DDACEDesignCompExp`, `FSUDesignCompExp`, and `PSUADEDesignCompExp`. 
void sample_to_variables ( const Real * sample_c_vars, Variables & vars ) [protected], [virtual]
convert column of samples array to variables; derived classes may reimplement for more than active continuous variables
   Default mapping that maps into continuous part of Variables only
   Reimplemented in NonDSampling.
   References Variables::adiv(), Variables::adrv(), Variables::all_discrete_int_variables(), Variables::all_discrete_real_variables(), Variables::continuous_variable(), Model::current_variables(), Variables::inactive_continuous_variables(), Variables::is_null(), Iterator::iteratedModel, Analyzer::numContinuousVars, and Variables::shared_data().
   Referenced by NonDLHSEvidence::post_process_samples(), Analyzer::pre_output(), Analyzer::samples_to_variables_array(), and Analyzer::update_best().

void initialize_run ( ) [protected], [virtual]
utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
   Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's initialize_run(), typically before performing its own implementation steps.
   Reimplemented from Iterator.
   Reimplemented in NonD.
   References Model::initialize_mapping(), Model::is_null(), Iterator::iteratedModel, Model::mapping_initialized(), Iterator::methodPCIter, Analyzer::resize(), Model::set_evaluation_reference(), and Iterator::summaryOutputFlag.
   Referenced by NonD::initialize_run().

void pre_run ( ) [protected], [virtual]
pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
   Pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically before performing its own implementation steps.
   Reimplemented from Iterator.
   Reimplemented in NonDLHSSampling, DDACEDesignCompExp, NonDRKDDarts, FSUDesignCompExp, ParamStudy, NonDMultilevelSampling, and PSUADEDesignCompExp.
   References Analyzer::bestVarsRespMap.
   Referenced by NonDMultilevelSampling::pre_run(), PSUADEDesignCompExp::pre_run(), ParamStudy::pre_run(), FSUDesignCompExp::pre_run(), NonDRKDDarts::pre_run(), DDACEDesignCompExp::pre_run(), and NonDLHSSampling::pre_run().

void post_run ( std::ostream & s ) [protected], [virtual]
post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s `post_run()`, typically *after* performing its own implementation steps.

Reimplemented from `Iterator`.

References `Model::is_null()`, `Iterator::iteratedModel`, `Model::print_evaluation_summary()`, `Analyzer::print_results()`, `Iterator::resultsDB`, `Iterator::summaryOutputFlag`, and `ResultsManager::write_databases()`.

Referred by `NonDMultilevelSampling::post_run()`, `PSUADesignCompExp::post_run()`, `ParamStudy::post_run()`, `DDACEDesignCompExp::post_run()`, `NonDLHSSampling::post_run()`, and `NonDRKDDarts::post_run()`.

```cpp
void finalize_run ( ) [protected], [virtual]
```
utility function to perform common operations following `post_run();` deallocation and resetting of instance pointers

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s `finalize_run()`, typically *after* performing its own implementation steps.

Reimplemented from `Iterator`.
Reimplemented in `NonD`.
References `Model::finalize_mapping()`, `Iterator::finalize_run()`, `Iterator::iteratedModel`, `Model::mapping_initialized()`, and `Analyzer::resize()`.

Referenced by `NonD::finalize_run()`.

```cpp
void pre_output ( ) [protected], [virtual]
```
Generate tabular output with active variables (compactMode) or all variables with their labels and response labels, with no data. `Variables` are sequenced \{cv, div, drv\}

Reimplemented from `Iterator`.
References `Analyzer::allSamples`, `Analyzer::allVariables`, `ParallelLibrary::command_line_pre_run_output()`, `ParallelLibrary::command_line_user_modes()`, `Analyzer::compactMode`, `Variables::copy()`, `Model::current_response()`, `Model::current_variables()`, `Model::interface_id()`, `Iterator::iteratedModel`, `Iterator::outputLevel`, `Iterator::parallelLib`, `Program-Options::pre_run_output_format()`, `ParallelLibrary::program_options()`, `Analyzer::sample_to_variables()`, `Dakota::write_precision`, `Variables::write_tabular()`, and `Analyzer::writePrecision`.

```cpp
void print_results ( std::ostream & s ) [protected], [virtual]
```
print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in `finalize_run()`.

Reimplemented from `Iterator`.
Reimplemented in `NonDGPMASBayesCalibration`, `NonDLHSSampling`, `NonDPolynomialChaos`, `NonDBayesCalibration`, `NonDREAMBayesCalibration`, `NonDPOFDarts`, `NonDLGlobalReliability`, `NonDVASABIBayesCalibration`, `NonDQUESTOBayesCalibration`, `NonDA ntiveSampling`, `NonDGImpSampling`, `NonDImapImpSampling`, `NonDExpansion`, `NonDInterval`, `NonDMultilevelSampling`, `PStudyDACE`, `Verification`, `NonDGlobalReliability`, and `RichExtrapVerification`.

References `Analyzer::bestVarsRespMap`, `ParamResponsePair::eval_id()`, `Response::function_values()`, `Analyzer::numLSqTerms`, `Analyzer::numObjFns`, `ParamResponsePair::response()`, and `ParamResponsePair::variables()`.

Referenced by `Analyzer::post_run()`, `Verification::print_results()`, `PStudyDACE::print_results()`, and `NonDLHSSampling::print_results()`.
13.4. ANALYZER CLASS REFERENCE

```cpp
const Model & algorithm::space_model() const [inline], [protected], [virtual]
```
default definition that gets redefined in selected derived Minimizers

Reimplemented from Iterator.

Reimplemented in NonDBayesCalibration, NonDExpansion, NonDGlobalInterval, and NonDReliability.

References Iterator::iteratedModel.

```cpp
void evaluate_parameter_sets ( Model & model, bool log resp flag, bool log best flag ) [protected]
```
perform function evaluations to map parameter sets (allVariables) into response sets (allResponses)

Convenience function for derived classes with sets of function evaluations to perform (e.g., NonDSampling, DDACEDesignCompExp, FSUDesignCompExp, ParamStudy).

References Iterator::activeSet, Analyzer::allHeaders, Analyzer::allResponses, Analyzer::allSamples, Analyzer::allVariables, Model::asynch_flag(), Analyzer::compactMode, Response::copy(), Model::current_response(), Model::current_variables(), Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), Model::synchronize(), Analyzer::update_best(), Analyzer::update_model_from_sample(), and Analyzer::update_model_from_variables().

Referenced by ParamStudy::core_run(), PSUADesignCompExp::core_run(), FSUDesignCompExp::core_run(), NonDAAdaptImpSampling::core_run(), DDACEDesignCompExp::core_run(), NonDLHSSampling::core_run(), NonDIntegration::core_run(), NonDSampling::core_run(), NonDSparseGrid::evaluate_grid_increment(), NonDSparseGrid::evaluate_set(), NonDMultilevelSampling::lf_increment(), NonDMultilevelSampling::multilevel_control_variate_mc_Qcorr(), NonDMultilevelSampling::multilevel_control_variate_mc_Ycorr(), NonDMultilevelSampling::multilevel_mc_Qsum(), NonDMultilevelSampling::multilevel_mc_Ysum(), NonDMultilevelSampling::shared_increment(), and NonDQUESTOBayesCalibration::update_model().

```cpp
void get_vbd_parameter_sets ( Model & model, int num_samples ) [protected]
```
generate replicate parameter sets for use in variance-based decomposition

Generate (numvars + 2)∗num_samples replicate sets for VBD, populating allSamples( numvars, (numvars + 2)∗num_samples )

References Dakota::abort_handler(), Analyzer::allSamples, Analyzer::compactMode, Analyzer::get_parameter_sets(), Analyzer::num_samples(), Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, and Analyzer::vary_pattern().

Referenced by FSUDesignCompExp::pre_run(), DDACEDesignCompExp::pre_run(), and NonDLHSSampling::pre_run().

```cpp
void compute_vbd_stats ( const int num_samples, const IntResponseMap & resp_samples ) [protected]
```
compute VBD-based Sobol indices

Calculation of sensitivity indices obtained by variance based decomposition. These indices are obtained by the Saltelli version of the Sobol VBD which uses (K+2)∗N function evaluations, where K is the number of dimensions (uncertain vars) and N is the number of samples.

References Dakota::abort_handler(), Analyzer::allSamples, Analyzer::num_samples(), Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, Analyzer::numFunctions, Analyzer::S4, and Analyzer::T4.

Referenced by FSUDesignCompExp::post_run(), DDACEDesignCompExp::post_run(), and NonDLHSSampling::post_run().
void read_variables_responses ( int num_evals, size_t num_vars ) [protected]

convenience function for reading variables/responses (used in derived classes post_input)

read num_evals variables/responses from file

References Dakota::abort_handler(), Analyzer::allResponses, Analyzer::allSamples, Analyzer::allVariables,
ParallelLibrary::command_line_post_run_input(), ParallelLibrary::command_line_user_modes(), Analyzer::compact-
Mode, Response::copy(), Variables::copy(), Model::current_response(), Model::current_variables(), Dakota::data-
pairs, ParamResponsePair::eval_id(), Model::evaluation_cache(), Iterator::iteratedModel, Model::manage_data-
recastings(), Analyzer::numLSqTerms, Analyzer::numObjFns, Iterator::outputLevel, Iterator::parallelLib, Program-
Options::post_run_input_format(), ParallelLibrary::program_options(), ParamResponsePair::response(), Model::restart-
_file(), Analyzer::update_best(), Model::user_space_to_iterator_space(), ParamResponsePair::variables(), Analyzer-
::variables_to_sample(), and ParallelLibrary::write_restart().

Referenced by PSUADEDesignCompExp::post_input(), ParamStudy::post_input(), FSUDesignCompExp::post-
_input(), DDACEDesignCompExp::post_input(), and NonDLHSSampling::post_input().

void print_sobol_indices ( std::ostream & s ) const [protected]

Printing of VBD results.

printing of variance based decomposition indices.

References Model::continuous_variable_labels(), Model::discrete_int_variable_labels(), Model::discrete_real-
variable_labels(), Iterator::iteratedModel, Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer-
::numDiscreteRealVars, Analyzer::numFunctions, Model::response_labels(), Analyzer::S4, Analyzer::T4, Analyzer-
::vbdDropTol, and Dakota::write_precision.

Referenced by PStudyDACE::print_results(), and NonDLHSSampling::print_results().

void variables_to_sample ( const Variables & vars, Real * sample_c_vars ) [protected], [virtual]

convert the active continuous variables into a column of allSamples

Default implementation maps active continuous variables only

Reimplemented in NonDSampling.

References Variables::continuous_variables(), and Analyzer::numContinuousVars.

Referenced by Analyzer::read_variables_responses(), and Analyzer::variables_array_to_samples().

The documentation for this class was generated from the following files:

- DakotaAnalyzer.hpp
- DakotaAnalyzer.cpp

### 13.5 ApplicationInterface Class Reference

Derived class within the interface class hierarchy for supporting interfaces to simulation codes.

Inheritance diagram for ApplicationInterface:
Public Member Functions

- **ApplicationInterface** (const ProblemDescDB &problem_db)
  constructor

- **~ApplicationInterface** ()
  destructor

Protected Member Functions

- void **init_communicators** (const IntArray &message_lengths, int max_eval_concurrency)
  allocate communicator partitions for concurrent evaluations within an iterator and concurrent multiprocessor analyses within an evaluation.

- void **set_communicators** (const IntArray &message_lengths, int max_eval_concurrency)
  set the local parallel partition data for an interface (the partitions are already allocated in ParallelLibrary).

- void **init_serial** ()

- int **asynch_local_evaluation_concurrency** () const
  return asynchLocalEvalConcurrency

- short **interface_synchronization** () const
  return interfaceSynchronization

- bool **evaluation_cache** () const
  return evalCacheFlag

- bool **restart_file** () const
  return evalCacheFlag

- void **map** (const Variables &vars, const ActiveSet &set, Response &response, bool asynch_flag=false)
  Provides a "mapping" of variables to responses using a simulation. Protected due to Interface letter-envelope idiom.

- void **manage_failure** (const Variables &vars, const ActiveSet &set, Response &response, int failed_eval_id)
  manages a simulation failure using abort/retry/recover/continuation

- const IntResponseMap & **synchronize** ()
executes a blocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns all jobs

- const IntResponseMap & synchronize_nowait ()
  executes a nonblocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns a partial set of completed jobs

- void serve_evaluations ()
  run on evaluation servers to serve the iterator master

- void stop_evaluation_servers ()
  used by the iterator master to terminate evaluation servers

- bool check_multiprocessor_analysis (bool warn)
  checks on multiprocessor analysis configuration

- bool check_asynchronous (bool warn, int max_eval_concurrency)
  checks on asynchronous configuration (for direct interfaces)

- bool check_multiprocessor_asynchronous (bool warn, int max_eval_concurrency)
  checks on asynchronous settings for multiprocessor partitions

- virtual void derived_map (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)
  Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.

- virtual void derived_map_asynch (const ParamResponsePair &pair)
  Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.

- virtual void wait_local_evaluations (PRPQueue &prp_queue)
  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.

- virtual void test_local_evaluations (PRPQueue &prp_queue)
  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version is nonblocking and will return without any completions if none are immediately available.

- virtual void init_communicators_checks (int max_eval_concurrency)
  perform construct-time error checks on the parallel configuration

- virtual void set_communicators_checks (int max_eval_concurrency)
  perform run-time error checks on the parallel configuration

- void master_dynamic_schedule_analyses ()
  blocking dynamic schedule of all analyses within a function evaluation using message passing

- void serve_analyses_synch ()
  serve the master analysis scheduler and manage one synchronous analysis job at a time

- virtual int synchronous_local_analysis (int analysis_id)
  Execute a particular analysis (identified by analysis_id) synchronously on the local processor. Used for the derived class specifics within ApplicationInterface::serve_analyses_synch().

Protected Attributes

- ParallelLibrary & parallelLib
  reference to the ParallelLibrary object used to manage MPI partitions for the concurrent evaluations and concurrent analyses parallelism levels

- bool suppressOutput
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flag for suppressing output on slave processors

- int evalCommSize
  size of evalComm
- int evalCommRank
  processor rank within evalComm
- int evalServerId
  evaluation server identifier
- bool eaDedMasterFlag
  flag for dedicated master partitioning at ea level
- int analysisCommSize
  size of analysisComm
- int analysisCommRank
  processor rank within analysisComm
- int analysisServerId
  analysis server identifier
- int numAnalysisServers
  current number of analysis servers
- bool multiProcAnalysisFlag
  flag for multiprocessor analysis partitions
- bool asynchLocalAnalysisFlag
  flag for asynchronous local parallelism of analyses
- int asynchLocalAnalysisConcurrency
  limits the number of concurrent analyses in asynchronous local scheduling and specifies hybrid concurrency when message passing
- int asynchLocalEvalConcSpec
  user specification for asynchronous local evaluation concurrency
- int asynchLocalAnalysisConcSpec
  user specification for asynchronous local analysis concurrency
- int numAnalysisDrivers
  the number of analysis drivers used for each function evaluation (from the analysis_drivers interface specification)
- IntSet completionSet
  the set of completed fn_eval_id’s populated by wait_local_evaluations() and test_local_evaluations()
- String failureMessage
  base message for managing failed evals; will be followed with more details in screen output

Private Member Functions

- bool duplication_detect (const Variables &vars, Response &response, bool asynch_flag)
  checks data pairs and beforeSynchCorePRPQueue to see if the current evaluation request has already been performed or queued
- void init_default_asv (size_t num_fns)
  initialize default ASV if needed; this is done at run time due to post-construct time Response size changes.
- void master_dynamic_schedule_evaluations ()
blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a dedicated
master partition; executes on iteratorComm master
• void peer_static_schedule_evaluations()

  blocking static schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition;
  executes on iteratorComm master
• void peer_dynamic_schedule_evaluations()

  blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition;
  executes on iteratorComm master
• void asynchronous_local_evaluations(PRQueue &prp_queue)

  perform all jobs in prp_queue using asynchronous approaches on the local processor
• void synchronous_local_evaluations(PRQueue &prp_queue)

  perform all jobs in prp_queue using synchronous approaches on the local processor
• void master_dynamic_schedule_evaluations_nowait()

  execute a nonblocking dynamic schedule in a master-slave partition
• void peer_static_schedule_evaluations_nowait()

  execute a nonblocking static schedule in a peer partition
• void peer_dynamic_schedule_evaluations_nowait()

  execute a nonblocking dynamic schedule in a peer partition
• void asynchronous_local_evaluations_nowait(PRQueue &prp_queue)

  launch new jobs in prp_queue asynchronously (if capacity is available), perform nonblocking query of all running
  jobs, and process any completed jobs (handles both local master- and local peer-scheduling cases)
• void broadcast_evaluation(const ParamResponsePair &pair)

  convenience function for broadcasting an evaluation over an evalComm
• void broadcast_evaluation(int fn_eval_id, const Variables &vars, const ActiveSet &set)

  convenience function for broadcasting an evaluation over an evalComm
• void send_evaluation(PRQueueIter &prp_it, size_t buff_index, int server_id, bool peer_flag)

  helper function for sending sendBuffers[buff_index] to server
• void receive_evaluation(PRQueueIter &prp_it, size_t buff_index, int server_id, bool peer_flag)

  helper function for processing recvBuffers[buff_index] within scheduler
• void launch_asynch_local(PRQueueIter &prp_it)

  launch an asynchronous local evaluation
• void process_asynch_local(int fn_eval_id)

  process a completed asynchronous local evaluation
• void process_synch_local(PRQueueIter &prp_it)

  process a completed synchronous local evaluation
• void assign_asynch_local_queue(PRQueue &local_prp_queue, PRQueueIter &local_prp_iter)

  helper function for creating an initial active local queue by launching asynch local jobs from local_prp_queue, as
  limited by server capacity
• void assign_asynch_local_queue_nowait(PRQueue &local_prp_queue, PRQueueIter &local_prp_iter)

  helper function for updating an active local queue by backfilling asynch local jobs from local_prp_queue, as limited
  by server capacity
• size_t test_local_backfill(PRQueue &assign_queue, PRQueueIter &assign_iter)

  helper function for testing active asynch local jobs and then backfilling
• size_t test_receives_backfill(PRQueueIter &assign_iter, bool peer_flag)
helper function for testing receive requests and then backfilling jobs

- void `serve_evaluations_synch()`
  serve the evaluation message passing schedulers and perform one synchronous evaluation at a time

- void `serve_evaluations_synch_peer()`
  serve the evaluation message passing schedulers and perform one synchronous evaluation at a time as part of the 1st peer

- void `serve_evaluations_asynch()`
  serve the evaluation message passing schedulers and manage multiple asynchronous evaluations

- void `serve_evaluations_asynch_peer()`
  serve the evaluation message passing schedulers and perform multiple asynchronous evaluations as part of the 1st peer

- void `set_evaluation_communicators(const IntArray &message_lengths)`
  convenience function for updating the local evaluation partition data following `ParallelLibrary::init_evaluation_communicators()`.

- void `set_analysis_communicators()`
  convenience function for updating the local analysis partition data following `ParallelLibrary::init_analysis_communicators()`.

- void `init_serial_evaluations()`
  set concurrent evaluation configuration for serial operations

- void `init_serial_analyses()`
  set concurrent analysis configuration for serial operations (e.g., for local executions on a dedicated master)

- const `ParamResponsePair & get_source_pair(const Variables &target_vars)`
  convenience function for the continuation approach in `manage_failure()` for finding the nearest successful "source" evaluation to the failed "target"

- void `continuation(const Variables &target_vars, const ActiveSet &set, Response &response, const ParamResponsePair &source_pair, int failed_eval_id)`
  performs a 0th order continuation method to step from a successful "source" evaluation to the failed "target".
  Invoked by `manage_failure()` for `failAction == "continuation"`.

- void `common_input_filtering(const Variables &vars)`
  common input filtering operations, e.g., mesh movement

- void `common_output_filtering(Response &response)`
  common output filtering operations, e.g., data filtering

**Private Attributes**

- int `worldSize`
  size of `MPI_COMM_WORLD`

- int `worldRank`
  processor rank within `MPI_COMM_WORLD`

- int `iteratorCommSize`
  size of `iteratorComm`

- int `iteratorCommRank`
  processor rank within `iteratorComm`

- bool `ieMessagePass`
  flag for message passing at the scheduling level

- int `numEvalServers`
current number of evaluation servers

- int numEvalServersSpec
  user specification for number of evaluation servers

- int procsPerEvalSpec
  user specification for processors per analysis servers

- bool eaMessagePass
  flag for message passing at ea scheduling level

- int numAnalysisServersSpec
  user spec for number of analysis servers

- int procsPerAnalysisSpec
  user specification for processors per analysis servers

- int lenVarsMessage
  length of a MPIPackBuffer containing a Variables object; computed in Model::init_communicators()

- int lenVarsActSetMessage
  length of a MPIPackBuffer containing a Variables object and an ActiveSet object; computed in Model::init_communicators()

- int lenResponseMessage
  length of a MPIPackBuffer containing a Response object; computed in Model::init_communicators()

- int lenPRPairMessage
  length of a MPIPackBuffer containing a ParamResponsePair object; computed in Model::init_communicators()

- short evalScheduling
  user specification of evaluation scheduling algorithm: {DEFAULT,MASTER,PEER_DYNAMIC,PEER_STATIC}. Used for manual overrides of auto-configure logic in ParallelLibrary::resolve_inputs().

- short analysisScheduling
  user specification of analysis scheduling algorithm: {DEFAULT,MASTER,PEER}. Used for manual overrides of the auto-configure logic in ParallelLibrary::resolve_inputs().

- int asynchLocalEvalConcurrency
  limits the number of concurrent evaluations in asynchronous local scheduling and specifies hybrid concurrency when message passing

- bool asynchLocalEvalStatic
  whether the asynchronous local evaluations are to be performed with a static schedule (default false)

- BitArray localServerAssigned
  array with one bit per logical "server" indicating whether a job is currently running on the server (used for asynch local static schedules)

- short interfaceSynchronization
  interface synchronization specification: synchronous (default) or asynchronous

- bool headerFlag
  used by synchronize_nowait to manage header output frequency (since this function may be called many times prior to any completions)

- bool asvControlFlag
  used to manage a user request to deactivate the active set vector control. true = modify the ASV each evaluation as appropriate (default); false = ASV values are static so that the user need not check them on each evaluation.

- bool evalCacheFlag
  used to manage a user request to deactivate the function evaluation cache (i.e., queries and insertions using the data_pairs cache).
- **bool nearbyDuplicateDetect**
  - flag indicating optional usage of tolerance-based duplication detection (less efficient, but helpful when experiencing restart cache misses)

- **Real nearbyTolerance**
  - tolerance value for tolerance-based duplication detection

- **bool restartFileFlag**
  - used to manage a user request to deactivate the restart file (i.e., insertions into write_restart).

- **SharedPtrData sharedRespData**
  - SharedResponseData of associated Response.

- **String gradientType**
  - type of gradients present in associated Response

- **String hessianType**
  - type of Hessians present in associated Response

- **IntSet gradMixedAnalyticIds**
  - IDs of analytic gradients when mixed gradients present.

- **IntSet hessMixedAnalyticIds**
  - IDs of analytic Hessians when mixed gradients present.

- **ShortArray defaultASV**
  - the static ASV values used when the user has selected asvControl = off

- **String failAction**
  - mitigation action for captured simulation failures: abort, retry, recover, or continuation

- **int failRetryLimit**
  - limit on the number of retries for the retry failAction

- **RealVector failRecoveryFnVals**
  - the dummy function values used for the recover failAction

- **IntResponseMap historyDuplicateMap**
  - used to bookkeep asynchronous evaluations which duplicate pair evaluations. Map key is evalIdCnt, map value is corresponding response.

- **std::map< PRPQueueHIter, Response > beforeSynchDuplicateMap**
  - used to bookkeep evalIdCnt, beforeSynchCorePRPQueue iterator, and response of asynchronous evaluations which duplicate queued beforeSynchCorePRPQueue evaluations

- **PRPQueue beforeSynchCorePRPQueue**
  - used to bookkeep vars/set/response of nonduplicate asynchronous core evaluations. This is the queue of jobs populated by asynchronous map() that is later scheduled in synchronize() or synchronize_nowait().

- **PRPQueue beforeSynchAlgPRPQueue**
  - used to bookkeep vars/set/response of asynchronous algebraic evaluations. This is the queue of algebraic jobs populated by asynchronous map() that is later evaluated in synchronize() or synchronize_nowait().

- **PRPQueue asynchLocalActivePRPQueue**
  - used by nonblocking asynchronous local schedulers to bookkeep active local jobs

- **std::map< int, IntSizetPair > msgPassRunningMap**
  - used by nonblocking message passing schedulers to bookkeep which jobs are running remotely

- **int nowaitEvalIdRef**
13.5.1 Detailed Description

Derived class within the interface class hierarchy for supporting interfaces to simulation codes.

ApplicationInterface provides an interface class for performing parameter to response mappings using simulation code(s). It provides common functionality for a number of derived classes and contains the majority of all of the scheduling algorithms in DAKOTA. The derived classes provide the specifics for managing code invocations using system calls, forks, direct procedure calls, or distributed resource facilities.

13.5.2 Member Function Documentation

void init_serial ( ) [inline], [protected], [virtual]

DataInterface.cpp defaults of 0 servers are needed to distinguish an explicit user request for 1 server (serialization of a parallelism level) from no user request (use parallel auto-config). This default causes problems when init_communicators() is not called for an interface object (e.g., static scheduling fails in DirectApplicationInterface::derived_map() for NestedModel::optionalInterface). This is the reason for this function: to reset certain defaults for interface objects that are used serially.

Reimplemented from Interface.

References ApplicationInterface::init_serial_analyses(), and ApplicationInterface::init_serial_evaluations().

void map ( const Variables & vars, const ActiveSet & set, Response & response, bool asynch_flag = false ) [protected], [virtual]

Provides a “mapping” of variables to responses using a simulation. Protected due to Interface letter-envelope idiom.

The function evaluator for application interfaces. Called from derived_evaluate() and derived_evaluate_nowait() in derived Model classes. If asynch_flag is not set, perform a blocking evaluation (using derived_map()). If asynch_flag is set, add the job to the beforeSynchCorePRPQueue queue for execution by one of the scheduler routines in synchronize() or synchronize_nowait(). Duplicate function evaluations are detected with duplication_detect().

Reimplemented from Interface.

References Response::active_set(), Interface::algebraic_mappings(), Interface::algebraicMappings, Interface::asv_mapping(), ApplicationInterface::asvControlFlag, ApplicationInterface::beforeSynchAlgPRPQueue, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::broadcast_evaluation(), Response::copy(), Interface::coreMappings, Interface::currEvalId, Dakota::data_pairs, ApplicationInterface::defaultASV, ApplicationInterface::derived_map(), ApplicationInterface::duplication_detect(), ApplicationInterface::evalCacheFlag, Interface::evalIdCntr, Interface::fineGrainEvalCounters, Interface::fnGradCounter, Interface::fnHessCounter, Interface::fnLabels, Interface::fnValCounter, Response::function_labels(), Interface::init_algebraic_mappings(), ApplicationInterface::init_default_asv(), Interface::init_evaluation_counters(), Interface::interfaceId, ApplicationInterface::manage_failure(), Interface::multiProcEvalFlag, Interface::newEvalIdCntr, Interface::newFnGradCounter, Interface::newFnHessCounter,
const IntResponseMap & synchronize() [protected], [virtual]

executes a blocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns all jobs.

This function provides blocking synchronization for all cases of asynchronous evaluations, including the local asynchronous case (background system call, nonblocking fork, & multithreads), the message passing case, and the hybrid case. Called from derived_synchronize() in derived Model classes.

Reimplemented from Interface.

References Interface::algebraic_mappings(), Interface::algebraicMappings, Interface::asv_mapping(), ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::asynchLocalEvalStatic, ApplicationInterface::asynchronous_local_evaluations(), ApplicationInterface::beforeSynchAlgPRPQueue, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::beforeSynchDuplicateMap, Interface::cachedResponseMap, Interface::coreMappings, ApplicationInterface::evalScheduling, ApplicationInterface::historyDuplicateMap, Interface::ieDedMasterFlag, ApplicationInterface::ieMessagePass, Interface::interfaceId, Interface::interfaceType, ApplicationInterface::master_dynamic_schedule_evaluations(), Interface::multiProcEvalFlag, Interface::outputLevel, ApplicationInterface::peer_dynamic_schedule_evaluations(), ApplicationInterface::peer_static_schedule_evaluations(), Interface::rawResponseMap, Interface::response_mapping(), and ApplicationInterface::sharedRespData.

const IntResponseMap & synchronize_nowait() [protected], [virtual]

executes a nonblocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns a partial set of completed jobs.

This function provides nonblocking synchronization for the local asynchronous case and selected nonblocking message passing schedulers. Called from derived_synchronize_nowait() in derived Model classes.

Reimplemented from Interface.

References Interface::algebraic_mappings(), Interface::algebraicMappings, Interface::asv_mapping(), ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::asynchLocalEvalStatic, ApplicationInterface::asynchronous_local_evaluations_nowait(), ApplicationInterface::beforeSynchAlgPRPQueue, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::beforeSynchDuplicateMap, Interface::cachedResponseMap, Interface::coreMappings, ParamResponsePair::eval_id(), ApplicationInterface::evalScheduling, ApplicationInterface::headerFlag, ApplicationInterface::historyDuplicateMap, Interface::ieDedMasterFlag, ApplicationInterface::ieMessagePass, Interface::interfaceId, Interface::interfaceType, Dakota::lookup_by_eval_id(), ApplicationInterface::master_dynamic_schedule_evaluations_nowait(), Interface::multiProcEvalFlag, Interface::outputLevel, ApplicationInterface::peer_dynamic_schedule_evaluations_nowait(), ApplicationInterface::peer_static_schedule_evaluations_nowait(), Interface::rawResponseMap, ParamResponsePair::response(), Interface::response_mapping(), ApplicationInterface::sharedRespData, and Response::update().

void serve_evaluations() [protected], [virtual]

run on evaluation servers to serve the iterator master.

Invoked by the serve() function in derived Model classes. Passes control to serve_evaluations_synch(), serve_evaluations_asynch(), serve_evaluations_synch_peer(), or serve_evaluations_asynch_peer() according to specified concurrency, partition, and scheduler configuration.

Reimplemented from Interface.

References ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::evalServerId, Interface::ieDedMasterFlag, ApplicationInterface::serve_evaluations_asynch(), ApplicationInterface::serve_evaluations_asynch peer(), ApplicationInterface::serve_evaluations_synch(), and ApplicationInterface::serve_evaluations_synch_peer().
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void stop_evaluation_servers() [protected], [virtual]
used by the iterator master to terminate evaluation servers
This code is executed on the iteratorComm rank 0 processor when iteration on a particular model is complete.
It sends a termination signal (tag = 0 instead of a valid fn_eval_id) to each of the slave analysis servers. NOTE:
This function is called from the Strategy layer even when in serial mode. Therefore, use iteratorCommSize to provide
appropriate fall through behavior.
Reimplemented from Interface.
References ParallelLibrary::bcast_e(), ParallelLibrary::free(), ParallelConfiguration::ie_parallel_Level(), Interface-
::ieDedMasterFlag, ParallelLibrary::isend_e(), ApplicationInterface::iteratorCommSize, Interface::multiProcEval-
Flag, ApplicationInterface::numEvalServers, Interface::outputLevel, ParallelLibrary::parallel_configuration(), and
ApplicationInterface::parallelLib.

void init_communicators_checks(int max_eval_concurrency) [protected], [virtual]
perform construct-time error checks on the parallel configuration
Override DirectApplicInterface definition if plug-in to allow batch processing in Plugin{Serial,Parallel}Direct-
ApplicInterface.cpp
Reimplemented in DirectApplicInterface, SysCallApplicInterface, and ProcessHandleApplicInterface.
Referenced by ApplicationInterface::init_communicators().

void set_communicators_checks(int max_eval_concurrency) [protected], [virtual]
perform run-time error checks on the parallel configuration
Override DirectApplicInterface definition if plug-in to allow batch processing in Plugin{Serial,Parallel}Direct-
ApplicInterface.cpp
Reimplemented in DirectApplicInterface, SerialDirectApplicInterface, ParallelDirectApplicInterface, SysCall-
ApplicInterface, and ProcessHandleApplicInterface.
Referenced by ApplicationInterface::set_communicators().

void master_dynamic_schedule_analyses() [protected]
blocking dynamic schedule of all analyses within a function evaluation using message passing
This code is called from derived classes to provide the master portion of a master-slave algorithm for the
dynamic scheduling of analyses among slave servers. It is patterned after master_dynamic_schedule_evaluations().
It performs no analyses locally and matches either serve_analyses_synch() or serve_analyses_asynch() on the slave
servers, depending on the value of asynchLocalAnalysisConcurrency. Dynamic scheduling assigns jobs in 2
passes. The 1st pass gives each server the same number of jobs (equal to asynchLocalAnalysisConcurrency).
The 2nd pass assigns the remaining jobs to slave servers as previous jobs are completed. Single- and multilevel
parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within
ParallelLibrary.
References ApplicationInterface::asynchLocalAnalysisConcurrency, ParallelLibrary::free(), ParallelLibrary-
::irecv_ea(), ParallelLibrary::isend_ea(), ApplicationInterface::numAnalysisDrivers, ApplicationInterface::num-
AnalysisServers, ApplicationInterface::parallelLib, ParallelLibrary::waitall(), and ParallelLibrary::waitsome().
Referenced by ProcessHandleApplicInterface::create_evaluation_process(), SysCallApplicInterface::create_,
evaluation_process(), and DirectApplicInterface::derived_map().

void serve_analyses_synch() [protected]
serve the master analysis scheduler and manage one synchronous analysis job at a time
This code is called from derived classes to run synchronous analyses on slave processors. The slaves receive requests (blocking receive), do local derived_map_ac’s, and return codes. This is done continuously until a termination signal is received from the master. It is patterned after serve_evaluations_synch().

References ApplicationInterface::analysisCommRank, ParallelLibrary::bcast_a(), ParallelLibrary::isend_ea(), ApplicationInterface::multiProcAnalysisFlag, ApplicationInterface::parallelLib, ParallelLibrary::recv_ea(), ApplicationInterface::synchronous_local_analysis(), and ParallelLibrary::wait().

Referenced by ProcessHandleApplicInterface::create_evaluation_process(), SysCallApplicInterface::create_evaluation_process(), and DirectApplicInterface::derived_map().

bool duplication_detect ( const Variables & vars, Response & response, bool asynch_flag ) [private]
checks data_pairs and beforeSynchCorePRPQueue to see if the current evaluation request has already been performed or queued.

Called from map() to check incoming evaluation request for duplication with content of data_pairs and beforeSynchCorePRPQueue. If duplication is detected, return true, else return false. Manage bookkeeping with history-DuplicateMap and beforeSynchDuplicateMap. Note that the list searches can get very expensive if a long list is searched on every new function evaluation (either from a large number of previous jobs, a large number of pending jobs, or both). For this reason, a user request for deactivation of the evaluation cache results in a complete bypass of duplication_detect(), even though a beforeSynchCorePRPQueue search would still be meaningful. Since the intent of this request is to streamline operations, both list searches are bypassed.

References Response::active_set(), ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::beforeSynchDuplicateMap, Response::copy(), Dakota::data_pairs, ParamResponsePair::eval_id(), Interface::evalIdCntr, ApplicationInterface::historyDuplicateMap, Interface::interfaceId, Dakota::lookup_by_val(), ApplicationInterface::nearbyDuplicateDetect, ApplicationInterface::nearbyTolerance, and Response::update().

Referenced by ApplicationInterface::map().

void init_default_asv ( size_t num_fns ) [private]
initialize default ASV if needed; this is done at run time due to post-construct time Response size changes.

If the user has specified active_set_vector as off, then map() uses a default ASV which is constant for all function evaluations (so that the user need not check the content of the ASV on each evaluation). Only initialized if needed and not already sized.

References ApplicationInterface::asvControlFlag, ApplicationInterface::defaultASV, ApplicationInterface::gradientType, ApplicationInterface::gradMixedAnalyticIds, ApplicationInterface::hessianType, and ApplicationInterface::hessMixedAnalyticIds.

Referenced by ApplicationInterface::map().

void master_dynamic_schedule_evaluations ( ) [private]
blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a dedicated master partition; executes on iteratorComm master.

This code is called from synchronize() to provide the master portion of a master-slave algorithm for the dynamic scheduling of evaluations among slave servers. It performs no evaluations locally and matches either serve_evaluations_synch() or serve_evaluations_asynch() on the slave servers, depending on the value of asynch-LocalEvalConcurrency. Dynamic scheduling assigns jobs in 2 passes. The 1st pass gives each server the same number of jobs (equal to asynchLocalEvalConcurrency). The 2nd pass assigns the remaining jobs to slave servers as previous jobs are completed and returned. Single- and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary.peer
References ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, Dakota::lookup_by_eval_id(), ApplicationInterface::numEvalServers, Interface::outputLevel, ApplicationInterface::parallelLib, ApplicationInterface::receive_evaluation(), ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ParallelLibrary::waitall(), and ParallelLibrary::waitsome().

Referenced by ApplicationInterface::synchronize().

**void peer_static_schedule_evaluations() [private]**

blocking static schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition; executes on iteratorComm master

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from synchronize() in order to manage a static schedule for cases where peer 1 must block when evaluating its local job allocation (e.g., single or multiprocessor direct interface evaluations). It matches serve_evaluations_peer() for any other processors within the first evaluation partition and serve_evaluations_{synch,asynch}() for all other evaluation partitions (depending on asynchLocalEvalConcurrency). It performs function evaluations locally for its portion of the job allocation using either asynchronous_local_evaluations() or synchronous_local_evaluations(). Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary. The iteratorCommRank 0 processor assigns the static schedule since it is the only processor with access to beforeSynchCorePRPQueue (it runs the iterator and calls synchronize). The alternate design of each peer selecting its own jobs using the modulus operator would be applicable if execution of this function (and therefore the job list) were distributed.

References ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::asynchronous_local_evaluations(), ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::numEvalServers, Interface::outputLevel, ApplicationInterface::parallelLib, ApplicationInterface::receive_evaluation(), ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ApplicationInterface::synchronous_local_evaluations(), and ParallelLibrary::waitall().

Referenced by ApplicationInterface::synchronize().

**void peer_dynamic_schedule_evaluations() [private]**

blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition; executes on iteratorComm master

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from synchronize() in order to manage a dynamic schedule, as enabled by nonblocking management of local asynchronous jobs. It matches serve_evaluations_{synch,asynch}() for other evaluation partitions, depending on asynchLocalEvalConcurrency; it does not match serve_evaluations_peer() since, for local asynchronous jobs, the first evaluation partition cannot be multiprocessor. It performs function evaluations locally for its portion of the job allocation using asynchronous_local_evaluations_nowait(). Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary.

References ApplicationInterface::assign_asynch_local_queue(), ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::msgPassRunningMap, ApplicationInterface::numEvalServers, Interface::outputLevel, ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ApplicationInterface::test_local_backfill(), and ApplicationInterface::test_receives_backfill().

Referenced by ApplicationInterface::synchronize().

**void asynchronous_local_evaluations ( PRPQueue & local_prp_queue ) [private]**

perform all jobs in prp_queue using asynchronous approaches on the local processor
This function provides blocking synchronization for the local asynch case (background system call, nonblocking fork, or threads). It can be called from `synchronize()` for a complete local scheduling of all asynchronous jobs or from `peer_{static,dynamic}_schedule_evaluations()` to perform a local portion of the total job set. It uses `derived_map_asynch()` to initiate asynchronous evaluations and `wait_local_evaluations()` to capture completed jobs, and mirrors the `master_dynamic_schedule_evaluations()` message passing scheduler as much as possible (`wait_local_evaluations()` is modeled after MPI_Waitsome()).

References ApplicationInterface::assign_asynch_local_queue(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::asynchLocalEvalStatic, ApplicationInterface::completionSet, ApplicationInterface::launch_asynch_local(), ApplicationInterface::localServerAssigned, Dakota::lookup_by_eval_id(), ApplicationInterface::numEvalServers, Interface::outputLevel, ApplicationInterface::process_asynch_local(), Interface::rawResponseMap, and ApplicationInterface::wait_local_evaluations().

Referenced by ApplicationInterface::peer_static_schedule_evaluations(), and ApplicationInterface::synchronize().

```cpp
void synchronous_local_evaluations ( PRPQueue & local_prp_queue ) [private]
```

perform all jobs in `prp_queue` using synchronous approaches on the local processor

This function provides blocking synchronization for the local synchronous case (foreground system call, blocking fork, or procedure call from `derived_map()`). It is called from `peer_static_schedule_evaluations()` to perform a local portion of the total job set.

References ApplicationInterface::broadcast_evaluation(), Interface::currEvalId, ApplicationInterface::derived_map(), ApplicationInterface::manage_failure(), Interface::multiProcEvalFlag, and ApplicationInterface::process_synch_local().

Referenced by ApplicationInterface::peer_static_schedule_evaluations(), and ApplicationInterface::peer_static_schedule_evaluations_nowait().

```cpp
void master_dynamic_schedule_evaluations_nowait ( ) [private]
```

execute a nonblocking dynamic schedule in a master-slave partition

This code is called from `synchronize_nowait()` to provide the master portion of a nonblocking master-slave algorithm for the dynamic scheduling of evaluations among slave servers. It performs no evaluations locally and matches either `serve_evaluations_synch()` or `serve_evaluations_asynch()` on the slave servers, depending on the value of `asynchLocalEvalConcurrency`. Dynamic scheduling assigns jobs in 2 passes. The 1st pass gives each server the same number of jobs (equal to `asynchLocalEvalConcurrency`). The 2nd pass assigns the remaining jobs to slave servers as previous jobs are completed. Single- and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within `ParallelLibrary`.

References Dakota::abort_handler(), ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::headerFlag, ApplicationInterface::msgPassRunningMap, ApplicationInterface::numEvalServers, ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, and ApplicationInterface::test_receives_backfill().

Referenced by ApplicationInterface::synchronize_nowait().

```cpp
void peer_static_schedule_evaluations_nowait ( ) [private]
```

execute a nonblocking static schedule in a peer partition

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from `synchronize_nowait()` in order to manage a nonblocking static schedule. It matches `serve_evaluations_synch()` for other evaluation partitions (`asynchLocalEvalConcurrency == 1`). It performs blocking local function evaluations, one at a time, for its portion of the static schedule and checks for remote completions in between each local completion. Therefore, unlike `peer_dynamic_schedule_evaluations_nowait()`, this scheduler will always return at least one job. Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive, with specific syntax as
encapsulated within \texttt{ParallelLibrary}. The iteratorCommRank 0 processor assigns the static schedule since it is the only processor with access to \texttt{beforeSynchCorePRPQueue} (it runs the iterator and calls synchronize). The alternate design of each peer selecting its own jobs using the modulus operator would be applicable if execution of this function (and therefore the job list) were distributed.


Referenced by ApplicationInterface::\texttt{synchronize\_nowait()}.

\begin{verbatim}
void peer\_dynamic\_schedule\_evaluations\_nowait ( ) [private]
execute a nonblocking dynamic schedule in a peer partition
This code runs on the iteratorCommRank 0 processor (the iterator) and is called from \texttt{synchronize\_nowait()} in order to manage a nonblocking static schedule. It matches \texttt{serve\_evaluations\_\{synch,asynch\}()} for other evaluation partitions (depending on \texttt{asynchLocalEvalConcurrency}). It performs nonblocking local function evaluations for its portion of the static schedule using \texttt{asynchronous\_local\_evaluations()}. Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive, with specific syntax as encapsulated within \texttt{ParallelLibrary}. The iteratorCommRank 0 processor assigns the dynamic schedule since it is the only processor with access to \texttt{beforeSynchCorePRPQueue} (it runs the iterator and calls synchronize). The alternate design of each peer selecting its own jobs using the modulus operator would be applicable if execution of this function (and therefore the job list) were distributed.


Referenced by ApplicationInterface::\texttt{synchronize\_nowait()}.

void asynchronous\_local\_evaluations\_nowait ( PRPQueue & local\_prp\_queue ) [private]
launch new jobs in \texttt{prp\_queue} asynchronously (if capacity is available), perform nonblocking query of all running jobs, and process any completed jobs (handles both local master- and local peer-scheduling cases)
This function provides nonblocking synchronization for the local asynch case (background system call, non-blocking fork, or threads). It is called from \texttt{synchronize\_nowait()} and passed the complete set of all asynchronous jobs (before\texttt{SynchCorePRPQueue}). It uses \texttt{derived\_map\_asynch()} to initiate asynchronous evaluations and \texttt{test\_local\_evaluations()} to capture completed jobs in nonblocking mode. It mirrors a nonblocking message passing scheduler as much as possible (\texttt{test\_local\_evaluations()} modeled after MPI\_Testsome()). The result of this function is \texttt{rawResponseMap}, which uses \texttt{eval\_id} as a key. It is assumed that the incoming \texttt{local\_prp\_queue} contains only active and new jobs - i.e., all completed jobs are cleared by \texttt{synchronize\_nowait()}.

Also supports asynchronous local evaluations with static scheduling. This scheduling policy specifically ensures that a completed asynchronous evaluation \texttt{eval\_id} is replaced with an equivalent one, modulo \texttt{asynchLocalEvalConcurrency}. In the nowait case, this could render some servers idle if evaluations don’t come in \texttt{eval\_id}
order or some evaluations are cancelled by the caller in between calls. If this function is called with unlimited
local eval concurrency, the static scheduling request is ignored.

References ApplicationInterface::assign_async_local_queue_nowait(), ApplicationInterface::asyncLocalActive-
PRPQueue, ApplicationInterface::asyncLocalEvalConcurrency, ApplicationInterface::asyncLocalEvalStatic, Application-
Interface::headerFlag, and ApplicationInterface::test_local_backfill().

Referenced by ApplicationInterface::synchronize_nowait().

void serve_evaluations_synch ( ) [private]

serve the evaluation message passing schedulers and perform one synchronous evaluation at a time

This code is invoked by serve_evaluations() to perform one synchronous job at a time on each slave/peer
server. The servers receive requests (blocking receive), do local synchronous maps, and return results. This is
done continuously until a termination signal is received from the master (sent via stop_evaluation_servers()).

References ParallelLibrary::bcast_e(), Interface::currEvalId, ApplicationInterface::derived_map(), Application-
Interface::evalCommRank, ParallelLibrary::send_ie(), ApplicationInterface::lenResponseMessage, Application-
Interface::lenVarActSetMessage, ApplicationInterface::manage_failure(), Interface::multiProcEvalFlag, Application-
Interface::parallelLib, ParallelLibrary::recv_ie(), MPIPackBuffer::reset(), ApplicationInterface::sharedRespData,
and ParallelLibrary::wait().

Referenced by ApplicationInterface::serve_evaluations().

void serve_evaluations_synch_peer ( ) [private]

serve the evaluation message passing schedulers and perform one synchronous evaluation at a time as part of the
1st peer

This code is invoked by serve_evaluations() to perform a synchronous evaluation in coordination with the
iteratorCommRank 0 processor (the iterator) for static schedules. The bcast() matches either the bcast() in
synchronous_local_evaluations(), which is invoked by peer_static_schedule_evaluations(), or the bcast() in map().

References ParallelLibrary::bcast_e(), Interface::currEvalId, ApplicationInterface::derived_map(), Application-
Interface::lenVarActSetMessage, ApplicationInterface::manage_failure(), ApplicationInterface::parallelLib, and
ApplicationInterface::sharedRespData.

Referenced by ApplicationInterface::serve_evaluations().

void serve_evaluations_asynch ( ) [private]

serve the evaluation message passing schedulers and manage multiple asynchronous evaluations

This code is invoked by serve_evaluations() to perform multiple asynchronous jobs on each slave/peer server.
The servers test for any incoming jobs, launch any new jobs, process any completed jobs, and return any results.
Each of these components is nonblocking, although the server loop continues until a termination signal is received
from the master (sent via stop_evaluation_servers()). In the master-slave case, the master maintains the correct
number of jobs on each slave. In the static scheduling case, each server is responsible for limiting concurrency
(since the entire static schedule is sent to the peers at start up).

References Dakota::abort_handler(), ApplicationInterface::asyncLocalActivePRPQueue, ApplicationInterface-
::asyncLocalEvalConcurrency, ParallelLibrary::bcast_e(), ApplicationInterface::completionSet, ApplicationInterface-
::derived_map_async(), ApplicationInterface::evalCommRank, Interface::interfaceId, ParallelLibrary::irecv_ie(),
ApplicationInterface::lenResponseMessage, ApplicationInterface::lenVarActSetMessage, Dakota::lookup_by_eval-
_id(), Interface::multiProcEvalFlag, ApplicationInterface::parallelLib, ParallelLibrary::recv_ie(), MPIUnpackBuffer-
::reset(), ParallelLibrary::send_ie(), ApplicationInterface::sharedRespData, ParallelLibrary::test(), and Application-
Interface::test_local_evaluations().

Referenced by ApplicationInterface::serve_evaluations().
void serve_evaluations_asynch_peer() [private]

serve the evaluation message passing schedulers and perform multiple asynchronous evaluations as part of the 1st peer.

This code is invoked by serve_evaluations() to perform multiple asynchronous jobs on multiprocessor slave/peer servers. It matches the multiProcEvalFlag bcasts in ApplicationInterface::asynchronous_local_evaluations().

References Dakota::abort_handler(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ParallelLibrary::bcast(), ApplicationInterface::completionSet, ApplicationInterface::derived_map_asynch(), Interface::interfaceId, ApplicationInterface::lenVarsActSetMessage, Dakota::lookup_by_eval_id(), ApplicationInterface::paralleLib, MPIUnpackBuffer::reset(), ApplicationInterface::sharedRespData, and ApplicationInterface::test_local_evaluations().

Referenced by ApplicationInterface::serve_evaluations().

The documentation for this class was generated from the following files:

- ApplicationInterface.hpp
- ApplicationInterface.cpp

### 13.6 Approximation Class Reference

Base class for the approximation class hierarchy.

Inheritance diagram for Approximation:

```plaintext
Approximation
<table>
<thead>
<tr>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>GaussProcApproximation</td>
</tr>
</tbody>
</table>
```

#### Public Member Functions

- **Approximation()**
  - default constructor
- **Approximation(ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)**
  - standard constructor for envelope
- **Approximation(const SharedApproxData &shared_data)**
  - alternate constructor
- **Approximation(const Approximation &approx)**
  - copy constructor
- **virtual ~Approximation()**
  - destructor
- **Approximation operator=(const Approximation &approx)**
  - assignment operator
- **virtual void build()**
  - builds the approximation from scratch
- **virtual void export_model(const String &fn_label="", const String &export_prefix="", const unsigned short export_format=NO_MODEL_FORMAT)**
  - exports the approximation
13.6. APPROXIMATION CLASS REFERENCE

- virtual void **rebuild** ()
  
  rebuilds the approximation incrementally
- virtual void **pop** (bool save_data)
  
  removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args)
- virtual void **push** ()
  
  restores state prior to previous pop()
- virtual void **finalize** ()
  
  finalize approximation by applying all remaining trial sets
- virtual void **store** (size_t index= NPOS)
  
  store current approximation state for later combination
- virtual void **restore** (size_t index= NPOS)
  
  restore previous approximation state
- virtual void **removeStored** (size_t index= NPOS)
  
  remove a stored approximation prior to combination
- virtual void **combine** (short corr_type, size_t swap_index)
  
  combine current approximation with previously stored approximation
- virtual Real **value** (const Variables &vars)
  
  retrieve the approximate function value for a given parameter vector
- virtual const RealVector & **gradient** (const Variables &vars)
  
  retrieve the approximate function gradient for a given parameter vector
- virtual const RealSymMatrix & **hessian** (const Variables &vars)
  
  retrieve the approximate function Hessian for a given parameter vector
- virtual Real **prediction_variance** (const Variables &vars)
  
  retrieve the variance of the predicted value for a given parameter vector
- virtual Real **value** (const RealVector & c_vars)
  
  retrieve the approximate function value for a given parameter vector
- virtual const RealVector & **gradient** (const RealVector & c_vars)
  
  retrieve the approximate function gradient for a given parameter vector
- virtual const RealSymMatrix & **hessian** (const RealVector & c_vars)
  
  retrieve the approximate function Hessian for a given parameter vector
- virtual Real **prediction_variance** (const RealVector & c_vars)
  
  retrieve the variance of the predicted value for a given parameter vector
- virtual bool **diagnostics_available** ()
  
  check if diagnostics are available for this approximation type
- virtual Real **diagnostic** (const String &metric_type)
  
  retrieve a single diagnostic metric for the diagnostic type specified
- virtual RealArray **cv_diagnostic** (const StringArray &metric_types, unsigned num_folds)
  
  retrieve diagnostic metrics for the diagnostic types specified, applying
- virtual void **primary_diagnostics** (int fn_index)
  
  compute and print all requested diagnostics and cross-validation
- virtual RealArray **challenge_diagnostic** (const StringArray &metric_types, const RealMatrix &challenge_points, const RealVector &challenge_responses)
  
  compute requested diagnostics for user provided challenge pts
• virtual void challenge_diagnostics (int fn_index, const RealMatrix &challenge_points, const RealVector &challenge_responses)
  compute and print all requested diagnostics for user provided challenge pts
• virtual RealVector approximation_coefficients (bool normalized) const
  return the coefficient array computed by build()/rebuild()
• virtual void approximation_coefficients (const RealVector &approx_coeffs, bool normalized)
  set the coefficient array from external sources, rather than computing with build()/rebuild()
• virtual void coefficient_labels (std::vector<std::string> &coeff_labels) const
  print the coefficient array computed in build()/rebuild()
• virtual void print_coefficients (std::ostream &s, bool normalized)
  print the coefficient array computed in build()/rebuild()
• virtual int min_coefficients () const
  return the minimum number of samples (unknowns) required to build the derived class approximation type in num-Vars dimensions
• virtual int recommended_coefficients () const
  return the recommended number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
• virtual int num_constraints () const
  return the number of constraints to be enforced via an anchor point
• virtual void clear_current ()
  clear current build data in preparation for next build
• int min_points (bool constraint_flag) const
  return the minimum number of points required to build the approximation type in numVars dimensions. Uses _coefficients() and num_constraints().
• int recommended_points (bool constraint_flag) const
  return the recommended number of samples to build the approximation type in numVars dimensions (default same as min_points)
• const Pecos::SurrogateData & approximation_data () const
  return approxData
• void add (const Pecos::SurrogateDataVars &sdv, bool anchor_flag)
  append to SurrogateData::varsData or assign to SurrogateData::anchorVars
• void add (const Variables &vars, bool anchor_flag, bool deep_copy)
  extract the relevant vectors from Variables and invoke add(RealVector&, IntVector&, RealVector&)
• void add (const Real *sample_cvars, bool anchor_flag, bool deep_copy)
  create a RealVector view and invoke add(RealVector&, empty, empty)
• void add (const RealVector &cvars, const IntVector &di_vars, const RealVector &dr_vars, bool anchor_flag, bool deep_copy)
  shared code among add(Variables&) and add(Real*): adds a new data point by either appending to SurrogateData::varsData or assigning to SurrogateData::anchorVars, as dictated by anchor_flag. Uses add_point() and add_anchor().
• void add (const Pecos::SurrogateDataResp &sdr, bool anchor_flag)
  append to SurrogateData::respData or assign to SurrogateData::anchorResp
• void add (const Response &response, int fn_index, bool anchor_flag, bool deep_copy)
  adds a new data point by either appending to SurrogateData::respData or assigning to SurrogateData::anchor-Resp, as dictated by anchor_flag. Uses add_point() and add_anchor().
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- **void add** (const RealMatrix &samplevars, const RealVector &sampleresp)
  
  add data from the provided samples and response matrices, assuming continuous variables and function values only

- **void pop_count** (size_t count)
  
  appends to popCountStack (number of entries to pop from end of SurrogateData::\{vars,resp\}Data, based on size of last data set appended)

- **void clear_all** ()
  
  clear all build data (current and history) to restore original state

- **void clear_anchor** ()
  
  clear SurrogateData::anchor\{Vars,Resp\}

- **void clear_data** ()
  
  clear SurrogateData::\{vars,resp\}Data

- **void clear_popped** ()
  
  clear popCountStack and SurrogateData::popped\{Vars,Resp\}Trials

- **void set_bounds** (const RealVector &c_l_bnds, const RealVector &c_u_bnds, const IntVector &di_l_bnds, const IntVector &di_u_bnds, const RealVector &dr_l_bnds, const RealVector &dr_u_bnds)
  
  set approximation lower and upper bounds (currently only used by graphics)

- **Approximation * approx_rep** () const
  
  returns approxRep for access to derived class member functions that are not mapped to the top Approximation level

Protected Member Functions

- **Approximation** (BaseConstructor, const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)
  
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

- **Approximation** (NoDBBaseConstructor, const SharedApproxData &shared_data)
  
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

Protected Attributes

- **RealVector approxGradient**
  
  gradient of the approximation returned by gradient()

- **RealSymMatrix approxHessian**
  
  Hessian of the approximation returned by hessian()

- **Pecos::SurrogateData approxData**
  
  contains the variables/response data for constructing a single approximation model (one response function)

- **SharedApproxData * sharedDataRep**
  
  contains the approximation data that is shared among the response set

- **String approxLabel**
  
  label for approximation, if applicable
Private Member Functions

- **Approximation \* get_approx** (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)
  
  Used only by the standard envelope constructor to initialize approxRep to the appropriate derived type.

- **Approximation \* get_approx** (const SharedApproxData &shared_data)
  
  Used only by the alternate envelope constructor to initialize approxRep to the appropriate derived type.

Private Attributes

- SizetArray popCountStack
  
  a stack managing the number of points previously added by calls to append() that can be removed by calls to pop()

- Approximation \* approxRep
  
  pointer to the letter (initialized only for the envelope)

- int referenceCount
  
  number of objects sharing approxRep

13.6.1 Detailed Description

Base class for the approximation class hierarchy.

The **Approximation** class is the base class for the response data fit approximation class hierarchy in DAKOTA. One instance of an **Approximation** must be created for each function to be approximated (a vector of Approximations is contained in ApproximationInterface). For memory efficiency and enhanced polymorphism, the approximation hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (**Approximation**) serves as the envelope and one of the derived classes (selected in **Approximation-::get_approx()**) serves as the letter.

13.6.2 Constructor & Destructor Documentation

**Approximation()**

default constructor

The default constructor is used in Array<Approximation> instantiations and by the alternate envelope constructor. approxRep is NULL in this case (problem_db is needed to build a meaningful **Approximation** object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

**Approximation ( ProblemDescDB & problem_db, const SharedApproxData & shared_data, const String & approx_label )**

standard constructor for envelope

Envelope constructor only needs to extract enough data to properly execute get_approx, since Approximation(-BaseConstructor, problem_db) builds the actual base class data for the derived approximations.

References Dakota::abort_handler(), Approximation::approxRep, and Approximation::get_approx().

**Approximation ( const SharedApproxData & shared_data )**

alternate constructor

This is the alternate envelope constructor for instantiations on the fly. Since it does not have access to problem_db, it utilizes the **NoDBBaseConstructor** constructor chain.

References Dakota::abort_handler(), Approximation::approxRep, and Approximation::get_approx().
Approximation (const Approximation & approx)
copy constructor
Copy constructor manages sharing of approxRep and incrementing of referenceCount.
References Approximation::approxRep, and Approximation::referenceCount.

~Approximation() [virtual]
destructor
Destructor decrements referenceCount and only deletes approxRep when referenceCount reaches zero.
References Approximation::approxRep, and Approximation::referenceCount.

Approximation (BaseConstructor, const ProblemDescDB & problem_db, const SharedApproxData & shared_data, const String & approx_label) [protected]
constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
This constructor is the one which must build the base class data for all derived classes. get_approx() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_approx() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ~Approximation).

Approximation (NoDBBaseConstructor, const SharedApproxData & shared_data) [protected]
constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
This constructor is the one which must build the base class data for all derived classes. get_approx() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_approx() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ~Approximation).

13.6.3 Member Function Documentation
Approximation operator= (const Approximation & approx)
assignment operator
References Approximation::approxRep, and Approximation::referenceCount.

void build() [virtual]
builds the approximation from scratch
This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.
Reimplemented in PecosApproximation, VPSApproximation, GaussProcApproximation, SurfpackApproximation, TaylorApproximation, and TANA3Approximation.
References Dakota::abort_handler(), Approximation::approxData, Approximation::approxRep, Approximation::build(), Approximation::min_points(), SharedApproxData::numVars, and Approximation::sharedDataRep.
Referenced by TANA3Approximation::build(), TaylorApproximation::build(), Approximation::build(), SurfpackApproximation::build(), GaussProcApproximation::build(), VPSApproximation::build(), PecosApproximation::build(), and Approximation::rebuild().
void export_model ( const String & fn_label = "", const String & export_prefix = "", const unsigned short export_format = NO_MODEL_FORMAT ) [virtual]

exports the approximation. This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.
Reimplemented in SurfpackApproximation.
References Approximation::approxRep, and Approximation::export_model().
Referenced by Approximation::export_model().

void rebuild ( ) [virtual]

rebuilds the approximation incrementally.
This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.
Reimplemented in PecosApproximation.
References Approximation::approxRep, Approximation::build(), and Approximation::rebuild().
Referenced by Approximation::rebuild().

void pop ( bool save_data ) [virtual]

removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args).
This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.
Reimplemented in PecosApproximation.
References Dakota::abort_handler(), Approximation::approxData, Approximation::approxRep, Approximation::pop(), and Approximation::popCountStack.
Referenced by Approximation::pop(), and PecosApproximation::pop().

void push ( ) [virtual]

restores state prior to previous pop().
This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.
Reimplemented in PecosApproximation.
References Approximation::approxData, Approximation::approxRep, Approximation::popCountStack, Approximation::push(), SharedApproxData::retrieval_index(), and Approximation::sharedDataRep.
Referenced by Approximation::push(), and PecosApproximation::push().

void finalize ( ) [virtual]

finalize approximation by applying all remaining trial sets.
This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.
Reimplemented in PecosApproximation.
References Approximation::approxData, Approximation::approxRep, Approximation::clear_popped(), SharedApproxData::finalization_index(), Approximation::finalize(), and Approximation::sharedDataRep.
Referenced by Approximation::finalize(), and PecosApproximation::finalize().
void clear_current( ) [inline], [virtual]
clear current build data in preparation for next build
   Redefined by TANA3Approximation to clear current data but preserve history.
   Reimplemented in TANA3Approximation.
   References Approximation::approxRep, Approximation::clear_all(), and Approximation::clear_current().
   Referenced by Approximation::clear_current().

void clear_all( ) [inline]
clear all build data (current and history) to restore original state
   Clears out any history (e.g., TANA3Approximation use for a different response function in NonDReliability).
   References Approximation::approxData, Approximation::approxRep, and Approximation::clear_all().
   Referenced by Approximation::clear_all(), and Approximation::clear_current().

Approximation * get approx ( ProblemDescDB & problem_db, const SharedApproxData & shared_data,
const String & approx_label ) [private]
Used only by the standard envelope constructor to initialize approxRep to the appropriate derived type.
   Used only by the envelope constructor to initialize approxRep to the appropriate derived type.
   References SharedApproxData::approxType, SharedApproxData::data_rep(), ProblemDescDB::get_bool(), and
   Dakota::strends().
   Referenced by Approximation::Approximation().

Approximation * get approx ( const SharedApproxData & shared_data ) [private]
Used only by the alternate envelope constructor to initialize approxRep to the appropriate derived type.
   Used only by the envelope constructor to initialize approxRep to the appropriate derived type.
   References SharedApproxData::approxType, SharedApproxData::data_rep(), and Dakota::strends().
The documentation for this class was generated from the following files:
   • DakotaApproximation.hpp
   • DakotaApproximation.cpp

13.7 ApproximationInterface Class Reference
Derived class within the interface class hierarchy for supporting approximations to simulation-based results.
   Inheritance diagram for ApproximationInterface:
Public Member Functions

- **ApproximationInterface** (ProblemDescDB &problem_db, const Variables &am_vars, bool am_cache, const String &am_interface_id, const StringArray &fn_labels)
  primary constructor
- **ApproximationInterface** (const String &approx_type, const UShortArray &approx_order, const Variables &am_vars, bool am_cache, const String &am_interface_id, size_t num_fns, short data_order, short output_level)
  alternate constructor for instantiations on the fly
- \textit{\sim}ApproximationInterface ()
destructor

Protected Member Functions

- void map (const Variables &vars, const ActiveSet &set, Response &response, bool asynch_flag=false)
  the function evaluator: provides an approximate "mapping" from the variables to the responses using function-Surfaces
- int minimum_points (bool constraint_flag) const
  returns the minimum number of samples required to build the functionSurfaces
- int recommended_points (bool constraint_flag) const
  returns the recommended number of samples recommended to build the functionSurfaces
- void approximation_function_indices (const IntSet &approx_fn_indices)
  set the (currently active) approximation function index set
- void update_approximation (const Variables &vars, const IntResponsePair &response_pr)
- void update_approximation (const RealMatrix &samples, const IntResponseMap &resp_map)
- void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map)
- void build_approximation (const RealVector &c_lbnds, const RealVector &c_ubnds, const IntVector &d_l_lbnds, const IntVector &d_l_ubnds, const IntVector &d_u_lbnds, const RealVector &d_l_u_lbnds, const RealVector &d_r_l_lbnds, const RealVector &d_r_u_lbnds)
- void export_approximation ()
- void rebuild_approximation (const BoolDeque &rebuild_deque)
- void pop_approximation (bool save_surr_data)
- void push_approximation ()
- bool push_available ()
  queries the approximation for the ability to retrieve a previous increment
- void finalize_approximation ()
  finalizes the approximation by applying all trial increments
- void store_approximation (size_t index=NPOS)
  move the current approximation into storage for later combination; the index of the stored approximation can be passed to allow replacement instead of augmentation (default is push\_back)
- void restore_approximation (size_t index=NPOS)
  return an approximation from storage; the index identifies a particular stored data set (default is pop\_back from stored)
- void remove_stored_approximation (size_t index=NPOS)
remove a stored approximation, due to redundancy with the current approximation, prior to combination (default for no index is pop_back)

- **void combine_approximation** (short corr_type)
  combine the current approximation with previously stored data sets

- **Real2DArray cv_diagnostics** (const StringArray &metrics, unsigned num_folds)
  approximation cross-validation quality metrics per response function

- **Real2DArray challenge_diagnostics** (const StringArray &metric_types, const RealMatrix &challenge_pts, const RealVector &challenge_resps)

- **void clear_current()**
  clears current data from an approximation interface

- **void clear_all()**
  clears all data from an approximation interface

- **void clear_popped()**
  clears bookkeeping for popped data sets from an approximation interface

- **SharedApproxData & shared_approximation()**
  retrieve the SharedApproxData within an ApproximationInterface

- **std::vector< Approximation > & approximations()**
  retrieve the Approximations within an ApproximationInterface

- **const Pecos::SurrogateData & approximation_data(size_t index)**
  retrieve the approximation data from a particular Approximation within an ApproximationInterface

- **const RealVectorArray & approximation_coefficients(bool normalized=false)**
  retrieve the approximation coefficients from each Approximation within an ApproximationInterface

- **void approximation_coefficients(const RealVectorArray &approx_coeffs, bool normalized=false)**
  set the approximation coefficients within each Approximation within an ApproximationInterface

- **const RealVector & approximation_variances(const Variables &vars)**
  retrieve the approximation variances from each Approximation within an ApproximationInterface

- **const IntResponseMap & synchronize()**
  recovers data from a series of asynchronous evaluations (blocking)

- **const IntResponseMap & synchronize_nowait()**
  recovers data from a series of asynchronous evaluations (nonblocking)

**Private Member Functions**

- **void mixed_add(const Variables &vars, const Response &response, bool anchor)**
  add variables/response data to functionSurfaces using a mixture of shallow and deep copies

- **void mixed_add(const Real *c_vars, const Response &response, bool anchor)**
  add variables/response data to functionSurfaces using a mixture of shallow and deep copies

- **void shallow_add(const Variables &vars, const Response &response, bool anchor)**
  add variables/response data to functionSurfaces using a shallow copy

- **void sample_to_variables(const Real *sample_c_vars, size_t num_cv, Variables &vars)**
  populate continuous variables within vars from sample_c_vars

- **void update_pop_counts(const IntResponseMap &resp_map)**
  append to the popCountStack within each of the functionSurfaces based on the active set definitions within resp_map

- **void read_challenge_points(bool active_only)**
  Load approximation test points from user challenge points file.
Private Attributes

- IntSet approxFnIndices
  for incomplete approximation sets, this array specifies the response function subset that is approximated
- SharedApproxData sharedData
  data that is shared among all functionSurfaces
- std::vector< Approximation > functionSurfaces
  list of approximations, one per response function
- RealVectorArray functionSurfaceCoeffs
  array of approximation coefficient vectors, one per response function
- RealVector functionSurfaceVariances
  vector of approximation variances, one value per response function
- String challengeFile
  data file for user-supplied challenge data (per interface, since may contain multiple responses)
- unsigned short challengeFormat
  tabular format of the challenge points file
- bool challengeActiveOnly
  whether to import active only
- RealMatrix challengePoints
  container for the challenge points data (variables only)
- RealMatrix challengeResponses
  container for the challenge points data (responses only)
- Variables actualModelVars
  copy of the actualModel variables object used to simplify conversion among differing variable views
- bool actualModelCache
  indicates usage of an evaluation cache by the actualModel
- String actualModelllInterfaceld
  the interface id from the actualModel used for ordered PRPCache lookups
- IntResponseMap beforeSynchResponseMap
  bookkeeping map to catalogue responses generated in map() for use in synchronize() and synchronize_nowait().
  This supports pseudo-asynchronous operations (approximate responses are always computed synchronously, but
  asynchronous virtual functions are supported through bookkeeping).

Additional Inherited Members

13.7.1 Detailed Description

Derived class within the interface class hierarchy for supporting approximations to simulation-based results.
ApproximationInterface provides an interface class for building a set of global/local/multipoint approxima-
tions and performing approximate function evaluations using them. It contains a list of Approximation objects,
one for each response function.
13.7. APPROXIMATIONINTERFACE CLASS REFERENCE

13.7.2 Member Function Documentation

void update_approximation ( const Variables & vars, const IntResponsePair & response_pr )
[protected], [virtual]
This function populates/replaces each Approximation::anchorPoint with the incoming variables/response data point.
   Reimplemented from Interface.
   References ApproximationInterface::actualModelCache, ApproximationInterface::actualModelInterfaceId, Dakota::data_pairs, Dakota::lookup_by_ids(), ApproximationInterface::mixed_add(), and ApproximationInterface::shallow_add().

void update_approximation ( const RealMatrix & samples, const IntResponseMap & resp_map )
[protected], [virtual]
This function populates/replaces each Approximation::currentPoints with the incoming variables/response arrays.
   Reimplemented from Interface.
   References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::actualModelInterfaceId, ApproximationInterface::actualModelVars, ApproximationInterface::approxFnIndices, Dakota::data_pairs, ApproximationInterface::functionSurfaces, Dakota::lookup_by_ids(), ApproximationInterface::mixed_add(), ApproximationInterface::sample_to_variables(), and ApproximationInterface::shallow_add().

void update_approximation ( const VariablesArray & vars_array, const IntResponseMap & resp_map )
[protected], [virtual]
This function populates/replaces each Approximation::currentPoints with the incoming variables/response arrays.
   Reimplemented from Interface.
   References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::actualModelInterfaceId, ApproximationInterface::approxFnIndices, Dakota::data_pairs, ApproximationInterface::functionSurfaces, Dakota::lookup_by_ids(), ApproximationInterface::mixed_add(), and ApproximationInterface::shallow_add().

void append_approximation ( const Variables & vars, const IntResponsePair & response_pr )
[protected], [virtual]
This function appends to each Approximation::currentPoints with one incoming variables/response data point.
   Reimplemented from Interface.
   References ApproximationInterface::actualModelCache, ApproximationInterface::actualModelInterfaceId, ApproximationInterface::approxFnIndices, Dakota::data_pairs, ApproximationInterface::functionSurfaces, Dakota::lookup_by_ids(), ApproximationInterface::mixed_add(), and ApproximationInterface::shallow_add().

void append_approximation ( const RealMatrix & samples, const IntResponseMap & resp_map )
[protected], [virtual]
This function appends to each Approximation::currentPoints with multiple incoming variables/response data points.
   Reimplemented from Interface.
   References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::actualModelInterfaceId, ApproximationInterface::actualModelVars, Dakota::data_pairs, Dakota::lookup_by_ids(), ApproximationInterface::mixed_add(), ApproximationInterface::sample_to_variables(), ApproximationInterface::shallow_add(), and ApproximationInterface::update_pop_counts().
void append_approximation ( const VariablesArray & vars_array, const IntResponseMap & resp_map ) [protected], [virtual]

This function appends to each Approximation::currentPoints with multiple incoming variables/response data points.

Reimplemented from Interface.

References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::actual-ModelInterfaceId, Dakota::data_pairs, Dakota::lookup_by_ids(), ApproximationInterface::mixed_add(), Approximation-Interface::shallow_add(), and ApproximationInterface::update_pop_counts().

void build_approximation ( const RealVector & c_l_bnds, const RealVector & c_u_bnds, const IntVector & d_i_l_bnds, const IntVector & d_i_u_bnds, const RealVector & d_r_l_bnds, const RealVector & d_r_u_bnds ) [protected], [virtual]

This function finds the coefficients for each Approximation based on the data passed through update_approximation() calls. The bounds are used only for graphics visualization.

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, SharedApproxData::build(), ApproximationInterface-::challengeFile, ApproximationInterface::challengePoints, ApproximationInterface::challengeResponses, Approximation-Interface::functionSurfaces, ApproximationInterface::read_challenge_points(), SharedApproxData::set_bounds(), and ApproximationInterface::sharedData.

void export_approximation ( ) [protected], [virtual]

This function calls export on each approximation

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, and ApproximationInterface::functionSurfaces.

void rebuild_approximation ( const BoolDeque & rebuild_deque ) [protected], [virtual]

This function updates the coefficients for each Approximation based on data increments provided by {update,append}-approximation().

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, ApproximationInterface::functionSurfaces, SharedApprox-Data::rebuild(), and ApproximationInterface::sharedData.

void pop_approximation ( bool save_surr_data ) [inline], [protected], [virtual]

This function removes data provided by a previous append_approximation() call, possibly different numbers for each function, or as specified in pop_count, which is assumed to be the same for all functions.

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, ApproximationInterface::functionSurfaces, SharedApprox-Data::pop(), and ApproximationInterface::sharedData.

void push_approximation ( ) [inline], [protected], [virtual]

This function updates the coefficients for each Approximation based on data increments provided by {update,append}-approximation().

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, ApproximationInterface::functionSurfaces, SharedApprox-Data::post_push(), SharedApproxData::pre_push(), and ApproximationInterface::sharedData.
void read_challenge_points ( bool active_only ) [private]

Load approximation test points from user challenge points file.
Challenge data defaults to active/inactive, but user can override to active only.
References ApproximationInterface::actualModelVars, ApproximationInterface::challengeActiveOnly, ApproximationInterface::challengeFile, ApproximationInterface::challengePoints, ApproximationInterface::challengeResponses, Variables::copy(), and ApproximationInterface::functionSurfaces.
Referenced by ApproximationInterface::build_approximation().

13.7.3 Member Data Documentation

std::vector<Approximation> functionSurfaces [private]
list of approximations, one per response function
This formulation allows the use of mixed approximations (i.e., different approximations used for different response functions), although the input specification is not currently general enough to support it.
Referenced by ApproximationInterface::append_approximation(), ApproximationInterface::approximation_coefficients(), ApproximationInterface::approximation_data(), ApproximationInterface::approximation_variances(), ApproximationInterface::build_approximation(), ApproximationInterface::clear_all(), ApproximationInterface::clear_current(), ApproximationInterface::clear_popped(), ApproximationInterface::combine_approximation(), ApproximationInterface::cv_diagnostics(), ApproximationInterface::export_approximation(), ApproximationInterface::finalize_approximation(), ApproximationInterface::map(), ApproximationInterface::minimum_points(), ApproximationInterface::mixed_add(), ApproximationInterface::push_approximation(), ApproximationInterface::read_challenge_points(), ApproximationInterface::rebuild_approximation(), ApproximationInterface::recommended_points(), ApproximationInterface::remove_stored_approximation(), ApproximationInterface::restore_approximation(), ApproximationInterface::shallow_add(), ApproximationInterface::store_approximation(), ApproximationInterface::update_approximation(), and ApproximationInterface::update_pop_counts().
The documentation for this class was generated from the following files:

- ApproximationInterface.hpp
- ApproximationInterface.cpp

13.8 APPSEvalMgr Class Reference

Evaluation manager class for APPSPACK.
Inherits Executor.

Public Member Functions

- APPSEvalMgr (Model &model)
  constructor
- ~APPSEvalMgr ()
  destructor
- bool isReadyForWork () const
tells APPS whether or not there is a processor available to perform a function evaluation
- bool submit (const int apps_tag, const HOPSPACK::Vector &apps_xtrial, const HOPSPACK::EvalRequestType apps_request)
  performs a function evaluation at APPS-provided x_in
• int recv (int &apps_tag, HOPSPACK::Vector &apps_f, HOPSPACK::Vector &apps_cEqs, HOPSPACK::-
  Vector &apps_cIneqs, string &apps_msg)
  returns a function value to APPS
• std::string getEvaluatorType (void) const
  return the type of the Dakota linked evaluator
• void printDebugInfo (void) const
  empty implementation of debug info needed to complete the interface
• void printTimingInfo (void) const
  empty implementation of timing info needed to complete the interface
• void set_asynch_flag (const bool dakotaAsynchFlag)
  publishes whether or not to do asynchronous evaluations
• void set_blocking_synch (const bool blockingSynchFlag)
  publishes whether or not APPS is operating synchronously
• void set_total_workers (const int numDakotaWorkers)
  publishes the number of processors available for function evaluations
• void set_constraint_map (std::vector<int> constraintMapIndices, std::vector<double> constr-
  MapMultipliers, std::vector<double> constraintMapOffsets)
  publishes constraint transformation

Private Attributes

• Model & iteratedModel
  reference to the APPSOptimizer’s model passed in the constructor
• bool modelAsynchFlag
  flag for asynchronous function evaluations
• bool blockingSynch
  flag for APPS synchronous behavior
• int numWorkersUsed
  number of processors actively performing function evaluations
• int numWorkersTotal
  total number of processors available for performing function evaluations
• std::vector<int> constrMapIndices
  map from Dakota constraint number to APPS constraint number
• std::vector<double> constrMapMultipliers
  multipliers for constraint transformations
• std::vector<double> constrMapOffsets
  offsets for constraint transformations
• RealVector xTrial
  trial iterate
• std::map<int, int> tagList
  map of DAKOTA eval id to APPS eval id (for asynchronous evaluations)
• std::map<int, RealVector> functionList
  map of APPS eval id to responses (for synchronous evaluations)
• IntResponseMap dakotaResponseMap
  map of DAKOTA responses returned by synchronize_nowait()
13.8.1 Detailed Description

Evaluation manager class for APPSPACK.

The APPSEvalMgr class is derived from APPSPACK’s Executor class. It implements the methods of that class in such a way that allows DAKOTA to manage the computation of responses instead of APPS. Iterate and response values are passed between Dakota and APPSPACK via this interface.

13.8.2 Constructor & Destructor Documentation

APPSEvalMgr ( Model & model )

constructor

Evaluation manager class for APPSPACK.

The APPSEvalMgr class is derived from APPSPACK’s Executor class. It implements the methods of that class in such a way that allows DAKOTA to manage the computation of responses instead of APPS. Iterate and response values are passed between Dakota and APPSPACK via this interface.

13.8.3 Member Function Documentation

bool isReadyForWork ( ) const

tells APPS whether or not there is a processor available to perform a function evaluation

Check to see if all processors available for function evaluations are being used. If not, tell APPS that one is available.

References APPSEvalMgr::numWorkersTotal, and APPSEvalMgr::numWorkersUsed.

bool submit ( const int apps_tag, const HOPSPACK::Vector & apps_xtrial, const HOPSPACK::EvalRequestType apps_request )

performs a function evaluation at APPS-provided x_in

Convert APPSPACK vector of variables to DAKOTA vector of variables and perform function evaluation asynchronously or not as specified in the DAKOTA input deck. If evaluation is asynchronous, map the dakota id to the APPS tag. If evaluation is synchronous, map the responses to the APPS tag.

References Model::current_response(), Model::current_variables(), Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), Response::function_values(), APPSEvalMgr::functionList, APPSEvalMgr::iteratedModel, APPSEvalMgr::modelAsynchFlag, APPSEvalMgr::numWorkersTotal, APPSEvalMgr::numWorkersUsed, and APPSEvalMgr::tagList.

int recv ( int & apps_tag, HOPSPACK::Vector & apps_f, HOPSPACK::Vector & apps_cEqs, HOPSPACK::Vector & apps_cIneqs, string & apps_msg )

returns a function value to APPS

Retrieve a set of response values, convert to APPS data structures, and return them to APPS. APPS tags are tied to corresponding responses using the appropriate (i.e., asynchronous or synchronous) map.

References APPSEvalMgr::blockingSynch, APPSEvalMgr::constrMapIndices, APPSEvalMgr::constrMapMultipliers, APPSEvalMgr::constrMapOffsets, APPSEvalMgr::dakotaResponseMap, APPSEvalMgr::functionList, APPSEvalMgr::iteratedModel, APPSEvalMgr::modelAsynchFlag, APPSEvalMgr::numWorkersUsed, Model::synchronize(), Model::synchronize_nowait(), and APPSEvalMgr::tagList.

The documentation for this class was generated from the following files:

- APPSEvalMgr.hpp
- APPSEvalMgr.cpp
13.9 APPSOptimizer Class Reference

Wrapper class for HOPSPACK.

Inheritance diagram for APPSOptimizer:

```
Iterate

Minimizer

Optimize

APPSOptimizer
```

Public Member Functions

- `APPSOptimizer (ProblemDescDB &problem_db, Model &model)`
- `APPSOptimizer (Model &model)`
  alternate constructor for on-the-fly instantiation without ProblemDescDB
- `APPSOptimizer ()`
  alternate constructor for even more rudimentary on-the-fly instantiation
- `~APPSOptimizer ()`
  destructor
- `void core_run ()`
  compute the optimal solution

Protected Member Functions

- `void set_apps_parameters ()`
  sets options for specific methods based on user specifications
- `void initialize_variables_and_constraints ()`
  initializes problem variables and constraints

Protected Attributes

- `int numTotalVars`
  Total across all types of variables.
- `HOPSPACK::ParameterList params`
  Pointer to APPS parameter list.
- `HOPSPACK::ParameterList * problemParams`
  Pointer to APPS problem parameter sublist.
- `HOPSPACK::ParameterList * linearParams`
  Pointer to APPS linear constraint parameter sublist.
13.9. APPS_OPTIMIZER CLASS REFERENCE

- HOPSPACK::ParameterList * mediatorParams
  Pointer to APPS mediator parameter sublist.
- HOPSPACK::ParameterList * citizenParams
  Pointer to APPS citizen/algorithm parameter sublist.
- APPSEvalMgr * evalMgr
  Pointer to the APPS evaluation manager object.
- std::vector<int> constraintMapIndices
  map from Dakota constraint number to APPS constraint number
- std::vector<double> constraintMapMultipliers
  multipliers for constraint transformations
- std::vector<double> constraintMapOffsets
  offsets for constraint transformations

Additional Inherited Members

13.9.1 Detailed Description

Wrapper class for HOPSPACK.

The APPSOptimizer class provides a wrapper for HOPSPACK, a Sandia-developed C++ library for generalized pattern search. HOPSPACK defaults to a coordinate pattern search but also allows for augmented search patterns. It can solve problems with bounds, linear constraints, and general nonlinear constraints. APPSOptimizer uses an APPSEvalMgr object to manage the function evaluations.

The user input mappings are as follows: output max_function_evaluations, constraint_tol initial_delta, contraction_factor, threshold_delta, solution_target, synchronization, merit_function, constraint_penalty, and smoothing_factor are mapped into HOPS's "Display", "Maximum Evaluations", "Active Tolerance"/"Nonlinear Active Tolerance", "Initial Step", "Contraction Factor", "Step Tolerance", "Objective Target", "Synchronous Evaluations", "Penalty Function", "Penalty Parameter", and "Penalty Smoothing Value" data attributes. Refer to the HOPS web site (https://software.sandia.gov/trac/hopspack) for additional information on HOPS objects and controls.

13.9.2 Member Function Documentation

void core_run() [virtual]

compute the optimal solution

core_run redefines the Optimizer virtual function to perform the optimization using HOPS. It first sets up the problem data, then executes minimize() on the HOPS optimizer, and finally catalogues the results.

Reimplemented from Iterator.

References Model::asynch_flag(), Iterator::bestResponseArray, Iterator::bestVariablesArray, APPSOptimizer::constraintMapIndices, APPSOptimizer::constraintMapMultipliers, APPSOptimizer::constraintMapOffsets, APPSOptimizer::evalMgr, Model::evaluation_capacity(), APPSOptimizer::initialize_variables_and_constraints(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, APPSOptimizer::numTotalVars, APPSOptimizer::params, APPSEvalMgr::set_asynch_flag(), and APPSEvalMgr::set_total_workers().

void set_apps_parameters() [protected]

sets options for specific methods based on user specifications

Set all of the HOPS algorithmic parameters as specified in the DAKOTA input deck. This is called at construction time.
References APPSOptimizer::citizenParams, Minimizer::constraintTol, APPSOptimizer::evalMgr, ProblemDescDB::get_real(), ProblemDescDB::get_string(), ProblemDescDB::is_null(), APPSOptimizer::linearParams, Iterator::maxEvalConcurrency, Iterator::maxFunctionEvals, APPSOptimizer::mediatorParams, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, Iterator::outputLevel, APPSOptimizer::params, Iterator::probDescDB, APPSOptimizer::problemParams, and APPSEvalMgr::set_blocking_synch().

Referenced by APPSOptimizer::APPSOptimizer().

```cpp
void initialize_variables_and_constraints() [protected]
```
initializes problem variables and constraints

Set the variables and constraints as specified in the DAKOTA input deck. This is done at run time.

References Minimizer::bigIntBoundSize, Minimizer::bigRealBoundSize, APPSOptimizer::constraintMapIndices, APPSOptimizer::constraintMapMultipliers, APPSOptimizer::constraintMapOffsets, APPSOptimizer::evalMgr, Iterator::iteratedModel, APPSOptimizer::linearParams, Minimizer::numContinuousVars, Minimizer::numDiscreteIntVars, Minimizer::numDiscreteRealVars, Minimizer::numDiscreteStringVars, Minimizer::numLinearEqConstraints, Minimizer::numLinearIneqConstraints, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, APPSOptimizer::numTotalVars, APPSOptimizer::problemParams, and APPSEvalMgr::set_constraint_map().

Referenced by APPSOptimizer::core_run().

The documentation for this class was generated from the following files:

- APPSOptimizer.hpp
- APPSOptimizer.cpp

### 13.10 ApreproWriter Class Reference

Utility used in derived write_core to write in aprepro format.

**Public Member Functions**

- template<typename ArrayType>
  ```cpp
  void operator() (std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array)
  ```

### 13.10.1 Detailed Description

Utility used in derived write_core to write in aprepro format.

The documentation for this class was generated from the following file:

- DakotaVariables.hpp

### 13.11 BaseConstructor Struct Reference

Dummy struct for overloading letter-envelope constructors.

**Public Member Functions**

- BaseConstructor (int=0)

  *C++ structs can have constructors.*
13.11.1 Detailed Description

Dummy struct for overloading letter-envelope constructors.

BaseConstructor is used to overload the constructor for the base class portion of letter objects. It avoids infinite recursion (Coplien p.139) in the letter-envelope idiom by preventing the letter from instantiating another envelope. Putting this struct here avoids circular dependencies.

The documentation for this struct was generated from the following file:

- dakota_global_defs.hpp

13.12 BootstrapSampler< Data > Class Template Reference

Actual bootstrap sampler implementation for common data types.

Inheritance diagram for BootstrapSampler< Data >:

```
BootstrapSampler< Data >
BootstrapSamplerBase< Data >
BootstrapSamplerWithGS< Data, Getter, Setter >
```

Public Member Functions

- BootstrapSampler (const Data &orig_data, size_t block_size=1)
  Constructor for the sampler.
- virtual ~BootstrapSampler ()
  Destructor.
- virtual void operator() (size_t num_samp, Data &bootstrapped_sample)

Protected Attributes

- size_t blockSize
  Size of the block defining a sample.

Additional Inherited Members

13.12.1 Detailed Description

template< typename Data > class Dakota::BootstrapSampler< Data >

Actual bootstrap sampler implementation for common data types.

Template requires the given type to support an STL-like interface, including a size method and begin and end methods returning random access iterators.
13.12.2 Member Function Documentation

virtual void operator() ( size_t num_samp, Data & bootstrapped_sample ) [inline], [virtual]

Implements BootstrapSamplerBase< Data >.
Reimplemented in BootstrapSamplerWithGS< Data, Getter, Setter >.
References BootstrapSampler< Data >::blockSize, BootstrapSamplerBase< Data >::bootstrapRNG, BootstrapSamplerBase< Data >::origData, and BootstrapSamplerBase< Data >::sampler.
The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

13.13 BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > > Class Template Reference

Bootstrap sampler that is specialized to allow for the bootstrapping of RealMatrix.

Inheritance diagram for BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >:

```
BootstrapSamplerBase< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >

BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >
```

Public Types

- typedef Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > MatType

  Convenience definition.

Public Member Functions

- BootstrapSampler (const MatType &orig_data, size_t block_size=1)

  Constructor for the sampler.
- virtual ~BootstrapSampler ()

  Destructor.
- virtual void operator() (size_t num_samp, MatType &bootstrapped_sample)

Protected Attributes

- size_t blockSize

  Size of the block defining a sample.
13.14. **BOOTSTRAPSAMPLERBASE< DATA > CLASS TEMPLATE REFERENCE**

**Additional Inherited Members**

13.13.1 Detailed Description

```cpp
template<typename OrdinalType, typename ScalarType>
class Dakota::BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >
```

Bootstrap sampler that is specialized to allow for the bootstrapping of RealMatrix.

13.13.2 Member Function Documentation

```cpp
virtual void operator() ( size_t num_samp, MatType & bootstrapped_sample ) [inline], [virtual]
```

Implements `BootstrapSamplerBase< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >`. References `BootstrapSampler< Data >::blockSize`, `BootstrapSamplerBase< Data >::bootstrapRNG`, `BootstrapSamplerBase< Data >::origData`, and `BootstrapSamplerBase< Data >::sampler`.

The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

13.14 **BootstrapSamplerBase< Data > Class Template Reference**

Base class/interface for the bootstrap sampler.

Inheritance diagram for BootstrapSamplerBase< Data >:

- BootstrapSamplerBase< Data >
- BootstrapSampler< Data >
- BootstrapSamplerWithGS< Data, Getter, Setter >

**Public Member Functions**

- **BootstrapSamplerBase** (size_t data_size, Data orig_data)
  Constructor for the bootstrap functor base.
- virtual ~BootstrapSamplerBase ()
  Destructor.
- virtual void operator() (size_t num_samp, Data &bootstrapped_sample)=0
  Generate and store a new boostrapped sample into bootstrapped_sample.
- virtual size_t getDataSize ()
  Obtain the number of samples used in the empirical distribution.
- virtual void operator() (Data &bootstrapped_sample)
  Generate and store an dataSize out of dataSize bootstrap sample.
- virtual Data operator() ()
  Return boostrapped sample.
CHAPTER 13. CLASS DOCUMENTATION

Static Public Member Functions

- static void set_seed (size_t seed)

Protected Attributes

- boost::random::uniform_int_distribution sampler
  
  Uniform distribution to provide samples from the empirical distribution.

- const size_t dataSize
  
  Size of the dataset defining the empirical distribution.

- Data origData
  
  Original data defining the empirical distribution TODO: Consider if it should be const (breaks Teuchos)

Static Protected Attributes

- static boost::random::mt19937 bootstrapRNG
  
  Random number generator to use for sampling.

13.14.1 Detailed Description

```
template<typename Data>
class Dakota::BootstrapSamplerBase<Data>
```

Base class/interface for the bootstrap sampler.

**BootstrapSamplerBase** defines the minimum interface for a bootstrap sampler and handles initialization of the random variate generation used by the bootstrap. Functor is templated on the data type, but does not actually define a data member.

13.14.2 Member Data Documentation

**boost::random::mt19937 bootstrapRNG**  [static], [protected]

Random number generator to use for sampling.

The bootstrap random number generator.

Referenced by BootstrapSampler<Data>::operator(), BootstrapSampler<Teuchos::SerialDenseMatrix<OrdinalType, ScalarType>>::operator(), and BootstrapSamplerWithGS<Data, Getter, Setter>::operator().

The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

13.15 BootstrapSamplerWithGS<Data, Getter, Setter> Class Template Reference

A derived sampler to allow for user specification of the accessor methods.

Inheritance diagram for BootstrapSamplerWithGS<Data, Getter, Setter>:
Public Member Functions

- **BootstrapSamplerWithGS** (const Data &orig_data, Getter getter_method, Setter setter_method)
  Constructor with extra arguments for the accessor methods.
- virtual ~BootstrapSamplerWithGS ()
  Destructor.
- virtual void operator() (size_t num_samp, Data &bootstrapped_sample)
  Generate and store a new boostrapped sample into bootstrapped_sample TODO: bounds checking.

Protected Attributes

- Getter **getterMethod**
  Function to obtain a single sample from a Data object. Function should take a Data object and an unsigned integer corresponding to a sample index and return the sample.
- Setter **setterMethod**
  Function to place a single sample into a Data object. Function should take a Data object and an unsigned integer corresponding to the sample index to set.

Additional Inherited Members

13.15.1 Detailed Description

template<typename Data, typename Getter, typename Setter> class Dakota::BootstrapSamplerWithGS<
Data, Getter, Setter >

A derived sampler to allow for user specification of the accessor methods.

The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

13.16 callback_data Struct Reference

Public Attributes

- double **rosen_cdv_upper_bd**
  upper bound value to pass through parser to callback function
13.16.1 Detailed Description

Data structure to pass application-specific values through Dakota back to the callback function, for example to convey late updates to bounds, initial points, etc., to Dakota.

The documentation for this struct was generated from the following file:

- library_mode.cpp

13.17 COLINApplication Class Reference

Inherits Application< colin::MO_MINLP2_problem >.

Public Member Functions

- COLINApplication ()
  
  Default constructor. Required by COLIN's ApplicationHandle creation.

- COLINApplication (Model &model)

  Constructor with Model (not presently used).

- ~COLINApplication ()

  Destructor.

- void set_problem (Model &model)

  Helper function called after default construction to extract problem information from the Model and set it for COLIN.

- void set_blocking_synch (const bool blockingSynchFlag)

  Publishes whether or not COLIN is operating synchronously.

- virtual utilib::Any spawn_evaluation_impl (const utilib::Any &domain, const colin::AppRequest::request_map_t &requests, utilib::seed_t &seed)

  Schedule one or more requests at specified domain point, returning a DAKOTA-specific evaluation tracking ID.

- virtual bool evaluation_available ()

  Check to see if there are any function values ready to be collected.

- virtual void perform_evaluation_impl (const utilib::Any &domain, const colin::AppRequest::request_map_t &requests, utilib::seed_t &seed, colin::AppResponse::response_map_t &colin_responses)

  Perform a function evaluation at t given point.

- virtual utilib::Any collect_evaluation_impl (colin::AppResponse::response_map_t &responses, utilib::seed_t &seed)

  Collect a completed evaluation from DAKOTA.

- virtual void colin_request_to_dakota_request (const utilib::Any &domain, const colin::AppRequest::request_map_t &requests, utilib::seed_t &seed)

  Helper function to convert evaluation request data from COLIN structures to DAKOTA structures.

- virtual void dakota_response_to_colin_response (const Response &dakota_response, colin::AppResponse::response_map_t &colin_responses)

  Helper function to convert evaluation response data from DAKOTA structures to COLIN structures.

- virtual bool map_domain (const utilib::Any &src, utilib::Any &native, bool forward=true) const

  Map the domain point into data type desired by this application context.
13.17. COLINAPPLICATION CLASS REFERENCE

Protected Attributes

- Model iteratedModel
  Shallow copy of the model on which COLIN will iterate.
- bool blockingSynch
  Flag for COLIN synchronous behavior (Pattern Search only).
- ActiveSet activeSet
  Local copy of model’s active set for convenience.
- std::vector<int> requestedEvals
  Evaluations queued for async evaluation.
- IntResponseMap dakota_responses
  Eval_id to response mapping to cache completed jobs.

13.17.1 Detailed Description

COLINApplication is a DAKOTA class that is derived from COLIN’s Application hierarchy. It redefines a variety of virtual COLIN functions to use the corresponding DAKOTA functions. This is a more flexible algorithm library interfacing approach than can be obtained with the function pointer approaches used by NPSOLOptimizer and SNLLOptimizer.

13.17.2 Member Function Documentation

void set_problem ( Model & model )

Helper function called after default construction to extract problem information from the Model and set it for COLIN.

Set variable bounds and linear and nonlinear constraints. This avoids using probDescDB, so it is called by both the standard and the on-the-fly COLINOptimizer constructors.

References Response::active_set(), COLINApplication::activeSet, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::current_response(), Model::cv(), Model::discrete_int_lower_bounds(), Model::discrete_int_sets(), Model::discrete_int_upper_bounds(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::div(), Model::drv(), Model::dsv(), COLINApplication::iteratedModel, Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_upper_bounds(), Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Model::num_functions(), Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), and Model::primary_response_fn_sense().

Referenced by COLINApplication::COLINApplication().

utilib::Any spawn_evaluation_impl ( const utilib::Any & domain, const colin::AppRequest::request_map_t & requests, utilib::seed_t & seed ) [virtual]

Schedule one or more requests at specified domain point, returning a DAKOTA-specific evaluation tracking ID.

Schedule one or more requests at specified domain point, returning a DAKOTA-specific evaluation tracking ID. This is only called by COLIN’s concurrent evaluator, which is only instantiated when the Model supports async evals. The domain point is guaranteed to be compatible with data type specified by map_domain(...)

References COLINApplication::colin_request_to_dakota_request(), Model::evaluate_nowait(), Model::evaluation_id(), and COLINApplication::iteratedModel.
bool evaluation_available() [virtual]

Check to see if there are any function values ready to be collected.

Check to see if any asynchronous evaluations have finished. This is only called by COLIN’s concurrent evaluator, which is only instantiated when the Model supports asynch evals.

References COLINApplication::blockingSynch, COLINApplication::dakota_responses, COLINApplication::iteratedModel, Model::synchronize(), and Model::synchronize_nowait().

void perform_evaluation_impl(const utilib::Any &domain, const colin::AppRequest::request_map_t &requests, utilib::seed_t &seed, colin::AppResponse::response_map_t &colin_responses) [virtual]

Perform a function evaluation at t given point.

Perform an evaluation at a specified domain point. Wait for and return the response. This is only called by COLIN’s serial evaluator, which is only instantiated when the Model does not support asynch evals. The domain point is guaranteed to be compatible with data type specified by map_domain(...)

References COLINApplication::colin_request_to_dakota_request(), Model::current_response(), COLINApplication::dakota_response_to_colin_response(), Model::evaluate(), and COLINApplication::iteratedModel.

utilib::Any collect_evaluation_impl(const colin::AppResponse::response_map_t &colin_responses, utilib::seed_t &seed) [virtual]

Collect a completed evaluation from DAKOTA.

Collect the next completed evaluation from DAKOTA. Always returns the evalid of the response returned.

References COLINApplication::dakota_response_to_colin_response(), and COLINApplication::dakota_responses.

void colin_request_to_dakota_request(const utilib::Any &domain, const colin::AppRequest::request_map_t &requests, utilib::seed_t &seed) [virtual]

Helper function to convert evaluation request data from COLIN structures to DAKOTA structures.

Map COLIN info requests to DAKOTA objectives and constraints.

References Model::continuous_variables(), Model::discrete_int_sets(), Model::discrete_int_variable(), Model::discrete_real_variable(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::discrete_string_variable(), Model::div(), Model::drv(), Model::dsv(), COLINApplication::iteratedModel, Model::num_functions(), and Dakota::set_index_to_value().

Referenced by COLINApplication::perform_evaluation_impl(), and COLINApplication::spawn_evaluation_impl().

void dakota_response_to_colin_response(const Response &dakota_response, colin::AppResponse::response_map_t &colin_responses) [virtual]

Helper function to convert evaluation response data from DAKOTA structures to COLIN structures.

Map DAKOTA objective and constraint values to COLIN response.

References Response::active_set_request_vector(), and Response::function_value().

Referenced by COLINApplication::collect_evaluation_impl(), and COLINApplication::perform_evaluation_impl().

bool map_domain(const utilib::Any &src, utilib::Any &native, bool forward = true) const [virtual]

Map the domain point into data type desired by this application context.
Map the domain point into data type desired by this application context (utilib::MixedIntVars). This data type can be exposed from the Any &domain presented to spawn and collect.

The documentation for this class was generated from the following files:

- COLINAApplication.hpp
- COLINAApplication.cpp

### 13.18 COLINOptimizer Class Reference

Wrapper class for optimizers defined using COLIN.

Inheritance diagram for COLINOptimizer:

```
COLINOptimizer
    |       
    v       
Minimizer
    |       
    v       
Optimizer
    |       
    v       
Iterator

Public Member Functions

- **COLINOptimizer** (ProblemDescDB &problem_db, Model &model)  
  *standard constructor*
- **COLINOptimizer** (const String &method_name, Model &model, int seed, int max_iter, int max_eval)  
  *alternate constructor for on-the-fly instantiations*
- **COLINOptimizer** (const String &method_name, Model &model)  
  *alternate constructor for Iterator instantiations by name*
- **~COLINOptimizer** ()  
  *destructor*
- void **reset** ()  
  *clears internal optimizer state*
- void **core_run** ()  
  *iterates the COLIN solver to determine the optimal solution*
- bool **returns_multiple_points** () const  
  *some COLIN methods can return multiple points*

Protected Member Functions

- void **solver_setup** (unsigned short method_name)  
  *convenience function for setting up the particular COLIN solver and appropriate Application*
- void **set_rng** (int seed)  
  *sets up the random number generator for stochastic methods*
• void setSolverParameters ()
  
  sets construct-time options for specific methods based on user specifications, including calling method-specific set
  functions
• void postRun (std::ostream &s)
  
  Get the final set of points from the solver. Look up responses and sort, first according to constraint violation, then
  according to function value.
• std::pair< bool, bool > colin_cache_lookup (const colin::AppResponse &colinResponse, Response &tmpResponseHolder)
  
  Retrieve response from Colin AppResponse, return pair indicating success for <objective, constraints>
• double constraintViolation (const Response &tmpResponseHolder)
  
  Compute constraint violation, based on nonlinear constraints in iteratedModel and provided Response data.

Protected Attributes

• short solverType
  
  COLIN solver sub-type as enumerated in COLINOptimizer.cpp.
• colin::SolverHandle colinSolver
  handle to the COLIN solver
• std::pair< colin::ApplicationHandle, COLINApplication * > colinProblem
  handle and pointer to the COLINApplication object
• colin::EvaluationManager_Base * colinEvalMgr
  pointer to the COLIN evalutaion manager object
• utilib::RNG * rng
  random number generator pointer
• bool blockingSynch
  
  the synchronization setting: true if blocking, false if nonblocking
• Real constraint_penalty
  Buffer to hold problem constraint_penalty parameter.
• bool constant_penalty
  Buffer to hold problem constant_penalty parameter.

Additional Inherited Members

13.18.1 Detailed Description

Wrapper class for optimizers defined using COLIN.

The COLINOptimizer class wraps COLIN, a Sandia-developed C++ optimization interface library. A variety
of COLIN optimizers are defined in COLIN and its associated libraries, including SCOLIB which contains the
optimization components from the old COLINY (formerly SGOPT) library. COLIN contains optimizers such as
genetic algorithms, pattern search methods, and other nongradient-based techniques. COLINOptimizer uses a
COLINApplication object to perform the function evaluations.

The user input mappings are as follows: max_iterations, max_function_evaluations, convergence-
tolerance, and solution_accuracy are mapped into COLIN’s max_iterations, max_function_evaluations_this_trial, function_value_tolerance, sufficient_objective_value properties. An outputLevel is mapped to COLIN’s output_level property and a setting of debug activates
output of method initialization and sets the COLIN debug attribute to 10000 for the DEBUG output level. Refer to [Hart, W.E., 2006] for additional information on COLIN objects and controls.

13.18.2 Constructor & Destructor Documentation

**COLINOptimizer ( ProblemDescDB & problem, Model & model )**

standard constructor

  Standard constructor.

  References ProblemDescDB::get_int(), ProblemDescDB::get_ushort(), Iterator::probDescDB, COLINOptimizer::set_rng(), COLINOptimizer::set_solver_parameters(), and COLINOptimizer::solver_setup().

**COLINOptimizer ( const String & method_name, Model & model, int seed, int max_iter, int max_eval )**

alternate constructor for on-the-fly instantiations

  Alternate constructor for on-the-fly instantiations.

  References Iterator::maxFunctionEvals, Iterator::maxIterations, Iterator::method_string_to_enum(), COLINOptimizer::set_rng(), COLINOptimizer::set_solver_parameters(), and COLINOptimizer::solver_setup().

**COLINOptimizer ( const String & method_name, Model & model )**

alternate constructor for Iterator instantiations by name

  Alternate constructor for Iterator instantiations by name.

  References Iterator::method_string_to_enum(), COLINOptimizer::set_solver_parameters(), and COLINOptimizer::solver_setup().

13.18.3 Member Function Documentation

**void core_run ( ) [virtual]**

iterates the COLIN solver to determine the optimal solution

  core_run redefines the Optimizer virtual function to perform the optimization using COLIN. It first sets up the problem data, then executes optimize() on the COLIN solver and finally catalogues the results.

  Reimplemented from Iterator.

  References Dakota::NPOS, Dakota::abort_handler(), Model::asynch_flag(), COLINOptimizer::blockingSynch, COLINOptimizer::colinEvalMgr, COLINOptimizer::colinProblem, COLINOptimizer::colinSolver, COLINOptimizer::constant_penalty, COLINOptimizer::constraint_penalty, Model::continuous_variables(), Model::discrete_int_sets(), Model::discrete_int_variables(), Model::discrete_real_variables(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::discrete_string_variables(), Model::evaluation_capacity(), Iterator::iteratedModel, Minimizer::numDiscreteIntVars, Minimizer::numDiscreteRealVars, Minimizer::numDiscreteStringVars, Iterator::outputLevel, Dakota::set_value_to_index(), and COLINOptimizer::solverType.

**bool returns_multiple_points ( ) const [virtual]**

some COLIN methods can return multiple points

  Designate which solvers can return multiple final points.

  Reimplemented from Iterator.

  References COLINOptimizer::solverType.
void solver_setup ( unsigned short method_name ) [protected]

convenience function for setting up the particular COLIN solver and appropriate Application
This convenience function is called by the constructors in order to instantiate the solver.
References COLINOptimizer::colinProblem, COLINOptimizer::colinSolver, COLINOptimizer::constant_penalty,
COLINOptimizer::constraint_penalty, ProblemDescDB::get_string(), Iterator::method_enum_to_string(), Iterator::
::probDescDB, and COLINOptimizer::solverType.
Referenced by COLINOptimizer::COLINOptimizer().

void set_rng ( int seed ) [protected]
sets up the random number generator for stochastic methods
Instantiate random number generator (RNG).
References COLINOptimizer::colinSolver, and COLINOptimizer::rng.
Referenced by COLINOptimizer::COLINOptimizer().

void set_solver_parameters ( ) [protected]
sets construct-time options for specific methods based on user specifications, including calling method-specific
set functions
Sets solver properties based on user specifications. Called at construction time.
References Model::asynch_flag(), COLINOptimizer::blockingSynch, COLINOptimizer::colinSolver,
COLINOptimizer::constant_penalty, COLINOptimizer::constraint_penalty, Iterator::convergenceTol, ProblemDescDB::
::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_real(), ProblemDescDB::get_sat(), ProblemDescDB::
::get_string(), ProblemDescDB::is_null(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, Iterator::max-
FunctionEvals, Iterator::maxIterations, Minimizer::numContinuousVars, Iterator::outputLevel, Iterator::probDesc-
DB, and COLINOptimizer::solverType.
Referenced by COLINOptimizer::COLINOptimizer().

void post_run ( std::ostream & s ) [protected], [virtual]
Get the final set of points from the solver Look up responses and sort, first according to constraint violation, then
according to function value.
Supplement Optimizer::post_run to first retrieve points from the Colin cache (or possibly the Dakota DB)
and rank them. When complete, this function will populate bestVariablesArray and bestResponsesArray with
iterator-space data, that is, in the context of the solver, leaving any further untransformation to Optimizer.
Reimplemented from Iterator.
References Iterator::bestResponseArray, Iterator::bestVariablesArray, COLINOptimizer::colin_cache_lookup(),
COLINOptimizer::colinProblem, COLINOptimizer::colinSolver, COLINOptimizer::constraintViolation(), Variables::
::continuous_variables(), Response::copy(), Variables::copy(), Model::current_response(), Model::current_variables(),
Model::discrete_int_sets(), Variables::discrete_int_variable(), Variables::discrete_real_variable(), Model::discrete_set-
::int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Variables::discrete_string-
::variable(), Response::function_values(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, Minimizer::num-
DiscreteIntVars, Minimizer::numDiscreteRealVars, Minimizer::numDiscreteStringVars, Iterator::numFinalSolutions,
Optimizer::numObjectiveFns, Minimizer::objective(), Optimizer::post_run(), Model::primary_response_fn_sense(),
Model::primary_response_fn_weights(), Minimizer::resize_best_resp_array(), Minimizer::resize_best_vars_array(),
Dakota::set_index_to_value(), COLINOptimizer::solverType, and Model::subordinate_model().
std::pair<bool, bool> colin_cache_lookup ( const colin::AppResponse & colinResponse, Response & tmpResponseHolder ) [protected]

Retrieve response from Colin AppResponse, return pair indicating success for <objective, constraints>
Encapsulated Colin Cache response extraction, which will ultimately become the default lookup. Might want to return separate vectors of function values and constraints for use in the sort, but not for now (least change). Return true if not needed or successful lookup.
References Response::function_value(), Minimizer::numNonlinearConstraints, and Optimizer::numObjective-Fns.
Referenced by COLINOptimizer::post_run().

double constraint_violation ( const Response & tmpResponseHolder ) [protected]

Compute constraint violation, based on nonlinear constraints in iteratedModel and provided Response data.
BMA TODO: incorporate constraint tolerance, possibly via elevating SurrBasedMinimizer::constraint_violation().
Always use iteratedModel to get the constraints; they are in the right space.
References Response::function_values(), Iterator::iteratedModel, Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), and Minimizer::numIterPrimaryFns.
Referenced by COLINOptimizer::post_run().
The documentation for this class was generated from the following files:
• COLINOptimizer.hpp
• COLINOptimizer.cpp

13.19 CollabHybridMetaIterator Class Reference

Meta-iterator for hybrid iteration using multiple collaborating optimization and nonlinear least squares methods.
Inheritance diagram for CollabHybridMetaIterator:

Public Member Functions
• CollabHybridMetaIterator (ProblemDescDB &problem_db)
  standard constructor
• CollabHybridMetaIterator (ProblemDescDB &problem_db, Model &model)
  alternate constructor
• ~CollabHybridMetaIterator ()
  destructor
 Protected Member Functions

- void core_run ()
  Performs the collaborative hybrid iteration.

- void derived_init_communicators (ParLevLIter pl_iter)
  derived class contributions to initializing the communicators associated with this Iterator instance

- void derived_set_communicators (ParLevLIter pl_iter)
  derived class contributions to setting the communicators associated with this Iterator instance

- void derived_free_communicators (ParLevLIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance

- IntIntPair estimate_partition_bounds ()
  estimate the minimum and maximum partition sizes that can be utilized by this Iterator

- const Variables & variables_results () const
  return the final solution from the collaborative iteration (variables)

- const Response & response_results () const
  return the final solution from the collaborative iteration (response)

 Private Attributes

- String hybridCollabType
  abo or hops

- StringArray methodStrings
  the list of method pointer or method name identifiers

- StringArray modelStrings
  the list of model pointer identifiers for method identification by name

- bool lightwtMethodCtor
  use of lightweight Iterator construction by name

- bool singlePassedModel
  use of constructor that enforces use of a single passed Model

- IteratorArray selectedIterators
  the set of iterators, one for each entry in methodStrings

- ModelArray selectedModels
  the set of models, one for each iterator

- Variables bestVariables
  best variables found in collaborative iteration

- Response bestResponse
  best response found in collaborative iteration

 Additional Inherited Members

13.19.1 Detailed Description

Meta-iterator for hybrid iteration using multiple collaborating optimization and nonlinear least squares methods.
This meta-iterator has two approaches to hybrid iteration: (1) agent-based using the ABO framework; (2) nonagent-based using the HOPSPACK framework.
The documentation for this class was generated from the following files:
13.20 CommandLineHandler Class Reference

Utility class for managing command line inputs to DAKOTA.

Inheritance diagram for CommandLineHandler:

```
GetLongOpt
```

```
CommandLineHandler
```

**Public Member Functions**

- **CommandLineHandler ()**
  - default constructor, requires check_usage() call for parsing
- **CommandLineHandler (int argc, char **argv, int world_rank)**
  - constructor with parsing
- **~CommandLineHandler ()**
  - destructor
- **void check_usage (int argc, char **argv)**
  - Verifies that DAKOTA is called with the correct command usage. Prints a descriptive message and exits the program if incorrect.
- **int read_restart_evals () const**
  - Returns the number of evaluations to be read from the restart file (as specified on the DAKOTA command line) as an integer instead of a const char*.
- **void usage (std::ostream &outfile=Cout) const**
  - Print usage information to outfile, conditionally on rank.

**Private Member Functions**

- **void initialize_options ()**
  - enrolls the supported command line inputs.
- **void output_helper (const std::string &message, std::ostream &os) const**
  - output only on Dakota worldRank 0 if possible

**Private Attributes**

- **int worldRank**
  - Rank of this process within Dakota’s allocation; manages conditional output.
Additional Inherited Members

13.20.1 Detailed Description
Utility class for managing command line inputs to DAKOTA. 

CommandLineHandler provides additional functionality that is specific to DAKOTA’s needs for the definition and parsing of command line options. Inheritance is used to allow the class to have all the functionality of the base class, GetLongOpt.

13.20.2 Member Function Documentation

void output_helper ( const std::string & message, std::ostream & os ) const  [private]
output only on Dakota worldRank 0 if possible
When there is a valid ParallelLibrary, output only on rank 0
References CommandLineHandler::worldRank.
Referenced by CommandLineHandler::check_usage().
The documentation for this class was generated from the following files:
- CommandLineHandler.hpp
- CommandLineHandler.cpp

13.21 CommandShell Class Reference
Utility class which defines convenience operators for spawning processes with system calls.

Public Member Functions

- CommandShell ()
  constructor
- ~CommandShell ()
  destructor
- CommandShell & operator<< (const char *cmd)
  appends cmd to sysCommand
- CommandShell & operator<<(const std::string &cmd)
  convenient operator: appends string to the commandString to be executed
- CommandShell & operator<<(CommandShell & (f)(CommandShell &))
  allows passing of the flush function to the shell using <<
- CommandShell & flush ()
  "flushes" the shell; i.e. executes the sysCommand
- void asynch_flag (const bool flag)
  set the asynchFlag
- bool asynch_flag () const
  get the asynchFlag
- void suppress_output_flag (const bool flag)
  set the suppressOutputFlag
- bool suppress_output_flag () const
  get the suppressOutputFlag
**Private Attributes**

- `std::string sysCommand`
  
  The command string that is constructed through one or more `<<` insertions and then executed by flush.

- `bool asynchFlag`
  
  Flags nonblocking operation (background system calls)

- `bool suppressOutputFlag`
  
  Flags suppression of shell output (no command echo)

**13.21.1 Detailed Description**

Utility class which defines convenience operators for spawning processes with system calls.

The `CommandShell` class wraps the C `system()` utility and defines convenience operators for building a command string and then passing it to the shell.

**13.21.2 Member Function Documentation**

`CommandShell & operator<<( const char * cmd ) [inline]`

appends cmd to sysCommand

- Convenient operator: appends string to the commandString to be executed
- References `CommandShell::sysCommand`.

`CommandShell & operator<<( CommandShell &(*)(CommandShell &)) [inline]`

allows passing of the flush function to the shell using `<<`

- Convenience operator: allows passing of the flush func to the shell via `<<`

`CommandShell & flush( )`

"flushes" the shell; i.e. executes the sysCommand

- Executes the sysCommand by passing it to system(). Appends "&" if asynchFlag is set (background system call) and echos the sysCommand to Cout if suppressOutputFlag is not set.
- References Dakota::abort_handler(), CommandShell::asynchFlag, CommandShell::suppressOutputFlag, and CommandShell::sysCommand.
- Referenced by Dakota::flush().
- The documentation for this class was generated from the following files:
  - CommandShell.hpp
  - CommandShell.cpp

**13.22 ConcurrentMetaIterator Class Reference**

Meta-iterator for multi-start iteration or pareto set optimization.

Inheritance diagram for ConcurrentMetaIterator:
Public Member Functions

- ConcurrentMetaIterator (ProblemDescDB &problem_db)
  standard constructor
- ConcurrentMetaIterator (ProblemDescDB &problem_db, Model &model)
  alternate constructor
- ~ConcurrentMetaIterator ()
  destructor

Protected Member Functions

- void pre_run ()
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()
  Performs the concurrent iteration by executing selectedIterator on iteratedModel multiple times in parallel for different parameter sets.
- void print_results (std::ostream &s)
  print the final iterator results
- void derived_init_communicators (ParLevLIter pl_iter)
  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)
  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance
- IntIntPair estimate_partition_bounds ()
  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- void initialize_iterator (int job_index)
  used by IteratorScheduler to set the starting data for a run
- void pack_parameters_buffer (MPIPackBuffer &send_buffer, int job_index)
  used by IteratorScheduler to pack starting data for an iterator run
- void unpack_parameters_initialize (MPIUnpackBuffer &recv_buffer, int job_index)
  used by IteratorScheduler to unpack starting data and initialize an iterator run
- void pack_results_buffer (MPIPackBuffer &send_buffer, int job_index)
  used by IteratorScheduler to pack results data from an iterator run
- void unpack_results_buffer (MPIUnpackBuffer &recv_buffer, int job_index)
void update_local_results (int job_index)
    used by IteratorScheduler to update local results arrays

const Model & algorithm_space_model () const
    return the result of any recasting or surrogate model recursion layered on top of iteratedModel by the derived Iterator ctor chain

Private Member Functions

void initialize_iterator (const RealVector &param_set)
    called by unpack_parameters_initialize(MPIUnpackBuffer) and initialize_iterator(int) to update iteratedModel and selectedIterator

void initialize_model ()
    initialize the iterated Model prior to Iterator instantiation and define param_set_len

Private Attributes

Iterator selectedIterator
    the iterator selected for concurrent iteration

RealVector initialPt
    the initial continuous variables for restoring the starting point in the Pareto set minimization

RealVectorArray parameterSets
    an array of parameter set vectors (either multistart variable sets or pareto multi-objective/least squares weighting sets) to be performed.

int paramSetLen
    length of each of the parameter sets associated with an iterator job (number of continuous variables for MULTI_START, number of objective fns for PARETO_SET)

int numRandomJobs
    number of randomly-generated parameter sets to evaluate

int randomSeed
    seed for random number generator for random samples

PRPArray prpResults
    1-d array of ParamResponsePair results corresponding to numIteratorJobs

Friends

class IteratorScheduler
    protect scheduler callback functions from general access

Additional Inherited Members

13.22.1 Detailed Description

Meta-iterator for multi-start iteration or pareto set optimization.

This meta-iterator maintains two concurrent iterator capabilities. First, a general capability for running an iterator multiple times from different starting points is provided (often used for multi-start optimization, but not restricted to optimization). Second, a simple capability for mapping the "pareto frontier" (the set of optimal
solutions in multiobjective formulations) is provided. This pareto set is mapped through running an optimizer multiple times for different sets of multiobjective weightings.

### 13.22.2 Member Function Documentation

**void pre\_run ( )** [protected], [virtual]

Pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

- Pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s pre\_run(), if implemented, typically before performing its own implementation steps.

Reimplemented from Iterator.

References Analyzer::all\_samples(), Iterator::all\_samples(), ParallelLibrary::bcast\_hs(), Model::continuous\_lower\_bounds(), Model::continuous\_upper\_bounds(), Model::continuous\_variables(), Dakota::copy\_data(), Model::estimate\_message\_lengths(), ConcurrentMetaIterator::initialPt, Iterator::iteratedModel, IteratorScheduler::iterator\_message\_lengths(), IteratorScheduler::iteratorComm\_Rank, IteratorScheduler::iteratorScheduling, IteratorScheduler::iteratorServer\_Id, MetaIterator::iterSched, IteratorScheduler::lead\_rank(), Model::message\_lengths(), Iterator::method\_Name, Iterator::method\_PCIter, IteratorScheduler::miPL\_Index, IteratorScheduler::num\_Iterator\_Jobs, IteratorScheduler::num\_Iterator\_Servers, ConcurrentMetaIterator::num\_Random\_Jobs, Iterator::parallel\_Lib, ConcurrentMetaIterator::parameter\_Sets, ConcurrentMetaIterator::param\_Set\_Len, ConcurrentMetaIterator::prp\_Results, ConcurrentMetaIterator::random\_Seed, and MPIPackBuffer::size().

**void print\_results ( std::ostream & s )** [protected], [virtual]

Print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize\_run().

Reimplemented from Iterator.

References Variables::continuous\_variables(), Variables::discrete\_int\_variables(), Variables::discrete\_real\_variables(), ParamResponsePair::eval\_id(), Iterator::methodName, ConcurrentMetaIterator::parameter\_Sets, ConcurrentMetaIterator::param\_Set\_Len, ConcurrentMetaIterator::prp\_Results, ParamResponsePair::response(), ParamResponsePair::variables(), and Response::write\_tabular().

The documentation for this class was generated from the following files:

- ConcurrentMetaIterator.hpp
- ConcurrentMetaIterator.cpp

### 13.23 CONMINOptimizer Class Reference

Wrapper class for the CONMIN optimization library.

Inheritance diagram for CONMINOptimizer:
Public Member Functions

- **CONMINOptimizer** (ProblemDescDB &problem_db, Model &model)
  - standard constructor
- **CONMINOptimizer** (const String &method_string, Model &model)
  - alternate constructor; construct without ProblemDescDB
- **~CONMINOptimizer** ()
  - destructor
- void **core_run** ()
  - core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Protected Member Functions

- void **initialize_run** ()
  - performs run-time set up

Private Member Functions

- void **initialize** ()
  - Shared constructor code.
- void **allocate_workspace** ()
  - Allocates workspace for the optimizer.
- void **deallocate_workspace** ()
  - Releases workspace memory.
- void **allocate_constraints** ()
  - Allocates constraint mappings.

Private Attributes

- int **conminInfo**
  - INFO from CONMIN manual.
- int **printControl**
  - IPRINT from CONMIN manual (controls output verbosity)
- Real **objFnValue**
  - value of the objective function passed to CONMIN
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- RealVector `constraintValues`
  array of nonlinear constraint values passed to CONMIN
- int `numConminNlnConstr`
  total number of nonlinear constraints seen by CONMIN
- int `numConminLinConstr`
  total number of linear constraints seen by CONMIN
- int `numConminConstr`
  total number of linear and nonlinear constraints seen by CONMIN
- SetArray `constraintMappingIndices`
  a container of indices for referencing the corresponding Response constraints used in computing the CONMIN constraints.
- RealArray `constraintMappingMultipliers`
  a container of multipliers for mapping the Response constraints to the CONMIN constraints.
- RealArray `constraintMappingOffsets`
  a container of offsets for mapping the Response constraints to the CONMIN constraints.
- int `N1`
  Size variable for CONMIN arrays. See CONMIN manual.
- int `N2`
  Size variable for CONMIN arrays. See CONMIN manual.
- int `N3`
  Size variable for CONMIN arrays. See CONMIN manual.
- int `N4`
  Size variable for CONMIN arrays. See CONMIN manual.
- int `N5`
  Size variable for CONMIN arrays. See CONMIN manual.
- int `NFDG`
  Finite difference flag.
- int `IPRINT`
  Flag to control amount of output data.
- int `ITMAX`
  Flag to specify the maximum number of iterations.
- double `FDCH`
  Relative finite difference step size.
- double `FDCHM`
  Absolute finite difference step size.
- double `CT`
  Constraint thickness parameter.
- double `CTMIN`
  Minimum absolute value of CT used during optimization.
- double `CTL`
  Constraint thickness parameter for linear and side constraints.
- double `CTLMIN`
  Minimum value of CTL used during optimization.
• double DELFUN
  Relative convergence criterion threshold.
• double DABFUN
  Absolute convergence criterion threshold.
• double * conminDesVars
  Array of design variables used by CONMIN (length N1 = numdv+2)
• double * conminLowerBnds
  Array of lower bounds used by CONMIN (length N1 = numdv+2)
• double * conminUpperBnds
  Array of upper bounds used by CONMIN (length N1 = numdv+2)
• double * S
  Internal CONMIN array.
• double * G1
  Internal CONMIN array.
• double * G2
  Internal CONMIN array.
• double * B
  Internal CONMIN array.
• double * C
  Internal CONMIN array.
• int * MS1
  Internal CONMIN array.
• double * SCAL
  Internal CONMIN array.
• double * DF
  Internal CONMIN array.
• double * A
  Internal CONMIN array.
• int * ISC
  Internal CONMIN array.
• int * IC
  Internal CONMIN array.

Additional Inherited Members

13.23.1 Detailed Description

Wrapper class for the CONMIN optimization library.

The CONMINOptimizer class provides a wrapper for CONMIN, a Public-domain Fortran 77 optimization library written by Gary Vanderplaats under contract to NASA Ames Research Center. The CONMIN User’s Manual is contained in NASA Technical Memorandum X-62282, 1978. CONMIN uses a reverse communication mode, which avoids the static member function issues that arise with function pointer designs (see NPSOL-Optimizer and SNLLOptimizer).

The user input mappings are as follows: max_iterations is mapped into CONMIN’s ITMAX parameter, max_function_evaluations is implemented directly in the core_run() loop since there is no CONMIN
parameter equivalent, `convergence_tolerance` is mapped into CONMIN's DELFUN and DABFUN parameters, `output verbosity` is mapped into CONMIN's IPRINT parameter (verbose: IPRINT = 4; quiet: IPRINT = 2), gradient mode is mapped into CONMIN's NFDG parameter, and finite difference step size is mapped into CONMIN's FDCH and FDCHM parameters. Refer to [Vanderplaats, 1978] for additional information on CONMIN parameters.

13.23.2 Member Function Documentation

```cpp
void core_run() [virtual]
```

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
Reimplemented from `Iterator`.
References CONMINOptimizer::A, Iterator::activeSet, CONMINOptimizer::B, Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::bigRealBoundSize, CONMINOptimizer::C, CONMINOptimizer::conminDesVars, CONMINOptimizer::conminInfo, CONMINOptimizer::conminLowerBnds, CONMINOptimizer::conminUpperBnds, CONMINOptimizer::constraintMappingIndices, CONMINOptimizer::constraintMappingMultipliers, CONMINOptimizer::constraintMappingOffsets, CONMINOptimizer::constraintValues, Model::continuous_variables(), Dakota::copy_data(), CONMINOptimizer::CT, CONMINOptimizer::CTL, CONMINOptimizer::CTLMIN, CONMINOptimizer::CTMIN, Model::current_response(), CONMINOptimizer::DABFUN, CONMINOptimizer::deallocate_workspace(), CONMINOptimizer::DELFUN, CONMINOptimizer::DF, Model::evaluate(), CONMINOptimizer::FDCH, CONMINOptimizer::FDCHM, Response::function_gradients(), Response::function_values(), CONMINOptimizer::G1, CONMINOptimizer::G2, Model::gradient_type(), CONMINOptimizer::IC, CONMINOptimizer::IPRINT, CONMINOptimizer::ISC, Iterator::iteratedModel, CONMINOptimizer::ITMAX, Model::linear_eq_constraint_coeffs(), Model::linear_ineq_constraint_coeffs(), Optimizer::localObjectiveRecast, Iterator::maxFunctionEvals, CONMINOptimizer::MS1, CONMINOptimizer::N1, CONMINOptimizer::N2, CONMINOptimizer::N3, CONMINOptimizer::N4, CONMINOptimizer::N5, CONMINOptimizer::NFDG, Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), CONMINOptimizer::numConminConstr, CONMINOptimizer::numConminNlnConstr, Minimizer::numContinuousVars, Minimizer::numFunctions, Optimizer::numObjectiveFs, CONMINOptimizer::objFnValue, Iterator::outputLevel, Model::primary_response_fn_sense(), ActiveSet::request_value(), ActiveSet::request_values(), CONMINOptimizer::S, CONMINOptimizer::SCAL, Minimizer::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

13.23.3 Member Data Documentation

```cpp
int conminInfo [private]
```

INFO from CONMIN manual.
Information requested by CONMIN: 1 = evaluate objective and constraints, 2 = evaluate gradients of objective and constraints.
Referenced by CONMINOptimizer::core_run(), and CONMINOptimizer::initialize().

```cpp
int printControl [private]
```

IPRINT from CONMIN manual (controls output verbosity)
Values range from 0 (nothing) to 4 (most output), 0 = nothing, 1 = initial and final function information, 2 = all of #1 plus function value and design vars at each iteration, 3 = all of #2 plus constraint values and direction vectors, 4 = all of #3 plus gradients of the objective function and constraints, 5 = all of #4 plus proposed design vector, plus objective and constraint functions from the 1-D search.
Referenced by CONMINOptimizer::initialize().
RealVector constraintValues [private]

array of nonlinear constraint values passed to CONMIN

This array must be of nonzero length and must contain only one-sided inequality constraints which are \( \leq 0 \) (which requires a transformation from 2-sided inequalities and equalities).

Referenced by CONMINOptimizer::allocate workspace(), and CONMINOptimizer::core run().

SizetArray constraintMappingIndices [private]

a container of indices for referencing the corresponding Response constraints used in computing the CONMIN constraints.

The length of the container corresponds to the number of CONMIN constraints, and each entry in the container points to the corresponding DAKOTA constraint.

Referenced by CONMINOptimizer::allocate constraints(), and CONMINOptimizer::core run().

RealArray constraintMappingMultipliers [private]

a container of multipliers for mapping the Response constraints to the CONMIN constraints.

The length of the container corresponds to the number of CONMIN constraints, and each entry in the container stores a multiplier for the DAKOTA constraint identified with constraintMappingIndices. These multipliers are currently +1 or -1.

Referenced by CONMINOptimizer::allocate constraints(), and CONMINOptimizer::core run().

RealArray constraintMappingOffsets [private]

a container of offsets for mapping the Response constraints to the CONMIN constraints.

The length of the container corresponds to the number of CONMIN constraints, and each entry in the container stores an offset for the DAKOTA constraint identified with constraintMappingIndices. These offsets involve inequality bounds or equality targets, since CONMIN assumes constraint allowables = 0.

Referenced by CONMINOptimizer::allocate constraints(), and CONMINOptimizer::core run().

int N1 [private]

Size variable for CONMIN arrays. See CONMIN manual.

\[ N1 = \text{number of variables} + 2 \]

Referenced by CONMINOptimizer::allocate workspace(), CONMINOptimizer::core run(), and CONMINOptimizer::initialize run().

int N2 [private]

Size variable for CONMIN arrays. See CONMIN manual.

\[ N2 = \text{number of constraints} + 2 \times (\text{number of variables}) \]

Referenced by CONMINOptimizer::allocate workspace(), and CONMINOptimizer::core run().

int N3 [private]

Size variable for CONMIN arrays. See CONMIN manual.

\[ N3 = \text{Maximum possible number of active constraints} \]

Referenced by CONMINOptimizer::allocate workspace(), and CONMINOptimizer::core run().
int N4 [private]
Size variable for CONMIN arrays. See CONMIN manual.

N4 = Maximum(N3, number of variables)
Referenced by CONMINOptimizer::allocate_workspace(), and CONMINOptimizer::core_run().

int N5 [private]
Size variable for CONMIN arrays. See CONMIN manual.

N5 = 2 * (N4)
Referenced by CONMINOptimizer::allocate_workspace(), and CONMINOptimizer::core_run().

double CT [private]
Constraint thickness parameter.

The value of CT decreases in magnitude during optimization.
Referenced by CONMINOptimizer::core_run(), and CONMINOptimizer::initialize().

double* S [private]
Internal CONMIN array.

Move direction in N-dimensional space.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMIN-Optimizer::deallocate_workspace().

double* G1 [private]
Internal CONMIN array.

Temporary storage of constraint values.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMIN-Optimizer::deallocate_workspace().

double* G2 [private]
Internal CONMIN array.

Temporary storage of constraint values.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMIN-Optimizer::deallocate_workspace().

double* B [private]
Internal CONMIN array.

Temporary storage for computations involving array S.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMIN-Optimizer::deallocate_workspace().

double* C [private]
Internal CONMIN array.

Temporary storage for use with arrays B and S.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMIN-Optimizer::deallocate_workspace().
int* MS1  [private]
Internal CONMIN array.
Temporary storage for use with arrays B and S.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

double* SCAL  [private]
Internal CONMIN array.
Vector of scaling parameters for design parameter values.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

double* DF  [private]
Internal CONMIN array.
Temporary storage for analytic gradient data.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

double* A  [private]
Internal CONMIN array.
Temporary 2-D array for storage of constraint gradients.
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

int* ISC  [private]
Internal CONMIN array.
Array of flags to identify linear constraints. (not used in this implementation of CONMIN)
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), CONMINOptimizer::deallocate_workspace(), and CONMINOptimizer::initialize_run().

int* IC  [private]
Internal CONMIN array.
Array of flags to identify active and violated constraints
Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), CONMINOptimizer::deallocate_workspace(), and CONMINOptimizer::initialize_run().
The documentation for this class was generated from the following files:

- CONMINOptimizer.hpp
- CONMINOptimizer.cpp

13.24  ConsoleRedirector Class Reference

Public Member Functions

- ConsoleRedirector (std::ostream *dakota_stream, std::ostream *default_dest)
Constructor taking a reference to the Dakota Cout/Cerr handle and a default destination to use when no redirection (or destruct)

- ~ConsoleRedirector()
  when the redirector stack is destroyed, it will rebind the output handle to the default ostream, then destroy open files

- void push_back()
  push back the default or repeat the last pushed file stream

- void push_back(const String &filename)
  push back a new output filestream, or repeat the last one if no filename change

- void pop_back()
  pop the last redirection

Protected Attributes

- std::ostream * & ostreamHandle
  The handle (target ostream) through which output is sent; typically dakota_cout or dakota_cerr. Will be rebound to specific streams as they are pushed or popped.

- std::ostream * defaultOStream
  initial stream to reset to when redirections are done (typically std::cout or std::cerr)

- std::vector< boost::shared_ptr<OutputWriter> > ostreamDestinations
  stack of redirections to OutputWriters; shared pointers are used to potentially share the same ostream at multiple levels

Private Member Functions

- ConsoleRedirector()
  default constructor is disallowed

- ConsoleRedirector (const ConsoleRedirector &)
  copy constructor is disallowed due

- const ConsoleRedirector & operator= (const ConsoleRedirector &)
  assignment is disallowed

13.24.1 Detailed Description

Component to manage a set of output or error redirections. Push operations may present a new filename, or none in order to preserve current binding to cout/cerr or file, but place an entry on the stack. Cout/Cerr are rebound as needed when a stream is destroyed on pop.

The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp
13.25 Constraints Class Reference

Base class for the variable constraints class hierarchy.

Inheritance diagram for Constraints:

```
Constraints
    MixedVarConstraints
    RelaxedVarConstraints
```

Public Member Functions

- `Constraints()`
  default constructor
- `Constraints(const ProblemDescDB &prob_db, const SharedVariablesData &svd)`
  standard constructor
- `Constraints(const SharedVariablesData &svd)`
  alternate constructor for instantiations on the fly
- `Constraints(const Constraints &con)`
  copy constructor
- `virtual ~Constraints()`
  destructor
- `Constraints (const Constraints &con)`
  assignment operator
- `virtual void write (std::ostream &s) const`
  write a variable constraints object to an std::ostream
- `virtual void read (std::istream &s)`
  read a variable constraints object from an std::istream
- `const RealVector &continuous_lower_bounds () const`
  return the active continuous variable lower bounds
- `Real continuous_lower_bound (size_t i) const`
  return an active continuous variable lower bound
- `void continuous_lower_bounds (const RealVector &cl_bnds)`
  set the active continuous variable lower bounds
- `void continuous_lower_bound (Real cl_bnd, size_t i)`
  set an active continuous variable lower bound
- `const RealVector &continuous_upper_bounds () const`
  return the active continuous variable upper bounds
- `Real continuous_upper_bound (size_t i) const`
  return an active continuous variable upper bound
- `void continuous_upper_bounds (const RealVector &cu_bnds)`
  set the active continuous variable upper bounds
- `void continuous_upper_bound (Real cu_bnd, size_t i)`
  set an active continuous variable upper bound
set an active continuous variable upper bound

- const IntVector & discrete_int_lower_bounds () const
  return the active discrete variable lower bounds

- int discrete_int_lower_bound (size_t i) const
  return an active discrete variable lower bound

- void discrete_int_lower_bounds (const IntVector &dil_bnds)
  set the active discrete variable lower bounds

- void discrete_int_lower_bound (int dil_bnd, size_t i)
  set an active discrete variable lower bound

- const IntVector & discrete_int_upper_bounds () const
  return the active discrete variable upper bounds

- int discrete_int_upper_bound (size_t i) const
  return an active discrete variable upper bound

- void discrete_int_upper_bounds (const IntVector &diu_bnds)
  set the active discrete variable upper bounds

- void discrete_int_upper_bound (int diu_bnd, size_t i)
  set an active discrete variable upper bound

- const RealVector & discrete_real_lower_bounds () const
  return the active discrete variable lower bounds

- Real discrete_real_lower_bound (size_t i) const
  return an active discrete variable lower bound

- void discrete_real_lower_bounds (const RealVector &drl_bnds)
  set the active discrete variable lower bounds

- void discrete_real_lower_bound (Real drl_bnd, size_t i)
  set an active discrete variable lower bound

- const RealVector & discrete_real_upper_bounds () const
  return the active discrete variable upper bounds

- Real discrete_real_upper_bound (size_t i) const
  return an active discrete variable upper bound

- void discrete_real_upper_bounds (const RealVector &dru_bnds)
  set the active discrete variable upper bounds

- void discrete_real_upper_bound (Real dru_bnd, size_t i)
  set an active discrete variable upper bound

- const RealVector & inactive_continuous_lower_bounds () const
  return the inactive continuous lower bounds

- void inactive_continuous_lower_bounds (const RealVector &icl_bnds)
  set the inactive continuous lower bounds

- const RealVector & inactive_continuous_upper_bounds () const
  return the inactive continuous upper bounds

- void inactive_continuous_upper_bounds (const RealVector &icu_bnds)
  set the inactive continuous upper bounds

- const IntVector & inactive_discrete_int_lower_bounds () const
  return the inactive discrete lower bounds
13.25. CONSTRAINTS CLASS REFERENCE

- **void inactive_discrete_int_lower_bounds** (const IntVector &idl_bnds)
  set the inactive discrete lower bounds
- **const IntVector & inactive_discrete_int_upper_bounds** () const
  return the inactive discrete upper bounds
- **void inactive_discrete_int_upper_bounds** (const IntVector &idiu_bnds)
  set the inactive discrete upper bounds
- **const RealVector & inactive_discrete_real_lower_bounds** () const
  return the inactive discrete lower bounds
- **void inactive_discrete_real_lower_bounds** (const RealVector &idrl_bnds)
  set the inactive discrete lower bounds
- **const RealVector & inactive_discrete_real_upper_bounds** () const
  return the inactive discrete upper bounds
- **void inactive_discrete_real_upper_bounds** (const RealVector &idru_bnds)
  set the inactive discrete upper bounds
- **const RealVector & all_continuous_lower_bounds** () const
  returns a single array with all continuous lower bounds
- **void all_continuous_lower_bounds** (const RealVector &acl_bnds)
  sets all continuous lower bounds using a single array
- **void all_continuous_lower_bound** (Real acl_bnd, size_t i)
  set a lower bound within the all continuous lower bounds array
- **const RealVector & all_continuous_upper_bounds** () const
  returns a single array with all continuous upper bounds
- **void all_continuous_upper_bounds** (const RealVector &acu_bnds)
  sets all continuous upper bounds using a single array
- **void all_continuous_upper_bound** (Real acu_bnd, size_t i)
  set an upper bound within the all continuous upper bounds array
- **const IntVector & all_discrete_int_lower_bounds** () const
  returns a single array with all discrete lower bounds
- **void all_discrete_int_lower_bounds** (const IntVector &adil_bnds)
  sets all discrete lower bounds using a single array
- **void all_discrete_int_lower_bound** (int adil_bnd, size_t i)
  set a lower bound within the all discrete lower bounds array
- **const IntVector & all_discrete_int_upper_bounds** () const
  returns a single array with all discrete upper bounds
- **void all_discrete_int_upper_bounds** (const IntVector &adiu_bnds)
  sets all discrete upper bounds using a single array
- **void all_discrete_int_upper_bound** (int adiu_bnd, size_t i)
  set an upper bound within the all discrete upper bounds array
- **const RealVector & all_discrete_real_lower_bounds** () const
  returns a single array with all discrete lower bounds
- **void all_discrete_real_lower_bounds** (const RealVector &adrl_bnds)
  sets all discrete lower bounds using a single array
- **void all_discrete_real_lower_bound** (Real adrl_bnd, size_t i)
  set a lower bound within the all discrete real lower bounds array
- **const RealVector & all_discrete_real_upper_bounds** () const
  returns a single array with all discrete upper bounds
- **void all_discrete_real_upper_bounds** (const RealVector &adru_bnds)
  sets all discrete upper bounds using a single array
- **void all_discrete_real_upper_bound** (Real adru_bnd, size_t i)
  set an upper bound within the all discrete real upper bounds array
set a lower bound within the all discrete lower bounds array

- const RealVector & all_discrete_real_upper_bounds() const
  returns a single array with all discrete upper bounds
- void all_discrete_real_upper_bounds(const RealVector &adru_bnds)
  sets all discrete upper bounds using a single array
- void all_discrete_real_upper_bound(Real adru_bnd, size_t i)
  set an upper bound within the all discrete upper bounds array

- size_t num_linear_ineq_constraints() const
  return the number of linear inequality constraints
- size_t num_linear_eq_constraints() const
  return the number of linear equality constraints
- const RealMatrix & linear_ineq_constraint_coeffs() const
  return the linear inequality constraint coefficients
- void linear_ineq_constraint_coeffs(const RealMatrix &lin_ineq_coeffs)
  set the linear inequality constraint coefficients
- const RealVector & linear_ineq_constraint_lower_bounds() const
  return the linear inequality constraint lower bounds
- void linear_ineq_constraint_lower_bounds(const RealVector &lin_ineq_l_bnds)
  set the linear inequality constraint lower bounds
- const RealVector & linear_ineq_constraint_upper_bounds() const
  return the linear inequality constraint upper bounds
- void linear_ineq_constraint_upper_bounds(const RealVector &lin_ineq_u_bnds)
  set the linear inequality constraint upper bounds
- const RealMatrix & linear_eq_constraint_coeffs() const
  return the linear equality constraint coefficients
- void linear_eq_constraint_coeffs(const RealMatrix &lin_eq_coeffs)
  set the linear equality constraint coefficients
- const RealVector & linear_eq_constraint_targets() const
  return the linear equality constraint targets
- void linear_eq_constraint_targets(const RealVector &lin_eq_targets)
  set the linear equality constraint targets

- size_t num_nonlinear_ineq_constraints() const
  return the number of nonlinear inequality constraints
- size_t num_nonlinear_eq_constraints() const
  return the number of nonlinear equality constraints
- const RealVector & nonlinear_ineq_constraint_lower_bounds() const
  return the nonlinear inequality constraint lower bounds
- void nonlinear_ineq_constraint_lower_bounds(const RealVector &nln_ineq_l_bnds)
  set the nonlinear inequality constraint lower bounds
- const RealVector & nonlinear_ineq_constraint_upper_bounds() const
  return the nonlinear inequality constraint upper bounds
- void nonlinear_ineq_constraint_upper_bounds(const RealVector &nln_ineq_u_bnds)
  set the nonlinear inequality constraint upper bounds
• const RealVector & nonlinear_eq_constraint_targets() const
  return the nonlinear equality constraint targets
• void nonlinear_eq_constraint_targets(const RealVector &nln_eq_targets)
  set the nonlinear equality constraint targets

Constraints copy() const
  for use when a deep copy is needed (the representation is not shared)

void shape()
  shape the lower/upper bound arrays based on sharedVarsData

void reshape(size_t num_nln_ineq_cons, size_t num_nln_eq_cons, size_t num_linc_ineq_cons, size_t num_linc_eq_cons, const SharedVariablesData &svd)
  reshape the linear/nonlinear/bound constraint arrays and the lower/upper bound arrays

void reshape()
  reshape the lower/upper bound arrays based on sharedVarsData

void reshape(size_t num_nln_ineq_cons, size_t num_nln_eq_cons, size_t num_linc_ineq_cons, size_t num_linc_eq_cons)
  reshape the linear/nonlinear constraint arrays

void inactive_view(short view2)
  sets the inactive view based on higher level (nested) context

bool is_null() const
  function to check constraintsRep (does this envelope contain a letter)

Protected Member Functions

• Constraints(BaseConstructor, const ProblemDescDB &problem_db, const SharedVariablesData &svd)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

• Constraints(BaseConstructor, const SharedVariablesData &svd)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

• void build_views()
  construct active/inactive views of all variables arrays

• void build_active_views()
  construct active views of all variables bounds arrays

• void build_inactive_views()
  construct inactive views of all variables bounds arrays

• void manage_linear_constraints(const ProblemDescDB &problem_db)
  perform checks on user input, convert linear constraint coefficient input to matrices, and assign defaults

Protected Attributes

• SharedVariablesData sharedVarsData
  configuration data shared from a Variables instance

• RealVector allContinuousLowerBnds
  a continuous lower bounds array combining continuous design, uncertain, and continuous state variable types (all view).
CHAPTER 13. CLASS DOCUMENTATION

- **RealVector** `allContinuousUpperBnds`
  a continuous upper bounds array combining continuous design, uncertain, and continuous state variable types (all view).

- **IntVector** `allDiscreteIntLowerBnds`
  a discrete lower bounds array combining discrete design and discrete state variable types (all view).

- **IntVector** `allDiscreteIntUpperBnds`
  a discrete upper bounds array combining discrete design and discrete state variable types (all view).

- **RealVector** `allDiscreteRealLowerBnds`
  a discrete lower bounds array combining discrete design and discrete state variable types (all view).

- **RealVector** `allDiscreteRealUpperBnds`
  a discrete upper bounds array combining discrete design and discrete state variable types (all view).

- **size_t** `numNonlinearIneqCons`
  number of nonlinear inequality constraints

- **size_t** `numNonlinearEqCons`
  number of nonlinear equality constraints

- **RealVector** `nonlinearIneqConLowerBnds`
  nonlinear inequality constraint lower bounds

- **RealVector** `nonlinearIneqConUpperBnds`
  nonlinear inequality constraint upper bounds

- **RealVector** `nonlinearEqConTargets`
  nonlinear equality constraint targets

- **size_t** `numLinearIneqCons`
  number of linear inequality constraints

- **size_t** `numLinearEqCons`
  number of linear equality constraints

- **RealMatrix** `linearIneqConCoeffs`
  linear inequality constraint coefficients

- **RealMatrix** `linearEqConCoeffs`
  linear equality constraint coefficients

- **RealVector** `linearIneqConLowerBnds`
  linear inequality constraint lower bounds

- **RealVector** `linearIneqConUpperBnds`
  linear inequality constraint upper bounds

- **RealVector** `linearEqConTargets`
  linear equality constraint targets

- **RealVector** `continuousLowerBnds`
  the active continuous lower bounds array view

- **RealVector** `continuousUpperBnds`
  the active continuous upper bounds array view

- **IntVector** `discreteIntLowerBnds`
  the active discrete lower bounds array view

- **IntVector** `discreteIntUpperBnds`
  the active discrete upper bounds array view
• RealVector discreteRealLowerBnds
  the active discrete lower bounds array view
• RealVector discreteRealUpperBnds
  the active discrete upper bounds array view
• RealVector inactiveContinuousLowerBnds
  the inactive continuous lower bounds array view
• RealVector inactiveContinuousUpperBnds
  the inactive continuous upper bounds array view
• IntVector inactiveDiscreteIntLowerBnds
  the inactive discrete lower bounds array view
• IntVector inactiveDiscreteIntUpperBnds
  the inactive discrete upper bounds array view
• RealVector inactiveDiscreteRealLowerBnds
  the inactive discrete lower bounds array view
• RealVector inactiveDiscreteRealUpperBnds
  the inactive discrete upper bounds array view

Private Member Functions

• Constraints * get_constraints (const ProblemDescDB &problem_db, const SharedVariablesData &svd)
  Used only by the constructor to initialize constraintsRep to the appropriate derived type.
• Constraints * get_constraints (const SharedVariablesData &svd) const
  Used by copy() to initialize constraintsRep to the appropriate derived type.

Private Attributes

• Constraints * constraintsRep
  pointer to the letter (initialized only for the envelope)
• int referenceCount
  number of objects sharing constraintsRep

13.25.1 Detailed Description

Base class for the variable constraints class hierarchy.

The Constraints class is the base class for the class hierarchy managing bound, linear, and nonlinear constraints. Using the variable lower and upper bounds arrays from the input specification, different derived classes define different views of this data. The linear and nonlinear constraint data is consistent in all views and is managed at the base class level. For memory efficiency and enhanced polymorphism, the variable constraints hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Constraints) serves as the envelope and one of the derived classes (selected in Constraints::get_constraints()) serves as the letter.
13.25.2 Constructor & Destructor Documentation

Constraints ( )

default constructor

The default constructor: constraintsRep is NULL in this case (a populated problem_db is needed to build a meaningful Constraints object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

Constraints ( const ProblemDescDB & problem_db, const SharedVariablesData & svd )

standard constructor

The envelope constructor only needs to extract enough data to properly execute get_constraints, since the constructor overloaded with BaseConstructor builds the actual base class data inherited by the derived classes.

References Dakota::abort_handler(), Constraints::constraintsRep, and Constraints::get_constraints().

Constraints ( const SharedVariablesData & svd )

alternate constructor for instantiations on the fly

Envelope constructor for instantiations on the fly. This constructor executes get_constraints(view), which invokes the default derived/base constructors, followed by a reshape() based on vars_comps.

References Dakota::abort_handler(), Constraints::constraintsRep, and Constraints::get_constraints().

Constraints ( const Constraints & con )

copy constructor

Copy constructor manages sharing of constraintsRep and incrementing of referenceCount.

References Constraints::constraintsRep, and Constraints::referenceCount.

~Constraints ( ) [virtual]

destructor

Destructor decrements referenceCount and only deletes constraintsRep when referenceCount reaches zero.

References Constraints::constraintsRep, and Constraints::referenceCount.

Constraints ( BaseConstructor, const ProblemDescDB & problem_db, const SharedVariablesData & svd ) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_constraints() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_constraints() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ~Constraints).

References Constraints::build_views(), Constraints::manage_linear_constraints(), and Constraints::shape().

Constraints ( BaseConstructor, const SharedVariablesData & svd ) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_constraints() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to
avoid recursion in the base class constructor calling `get_constraints()` again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in `~Constraints`). References Constraints::build_views(), and Constraints::shape().

13.25.3 Member Function Documentation

**Constraints operator= ( const Constraints & con )**

assignment operator


  References Constraints::constraintsRep, and Constraints::referenceCount.

**Constraints copy ( ) const**

for use when a deep copy is needed (the representation is *not* shared)

  Deep copies are used for history mechanisms that catalogue permanent copies (should not change as the representation within userDefinedConstraints changes).

  References Constraints::allContinuousLowerBnds, Constraints::allContinuousUpperBnds, Constraints::allDiscrete-IntLowerBnds, Constraints::allDiscreteIntUpperBnds, Constraints::allDiscreteRealLowerBnds, Constraints::allDiscreteRealUpperBnds, Constraints::build_views(), Constraints::constraintsRep, Constraints::get_constraints(), Constraints::linearEqConCoeffs, Constraints::linearEqConTargets, Constraints::linearIneqConCoeffs, Constraints::linearIneqConLowerBnds, Constraints::linearIneqConUpperBnds, Constraints::nonlinearEqConTargets, Constraints::nonlinearEqConCoeffs, Constraints::nonlinearIneqConLowerBnds, Constraints::nonlinearIneqConUpperBnds, Constraints::numLinearEqCons, Constraints::numNonlinearEqCons, Constraints::numNonlinearIneqCons, and Constraints::sharedVarsData.

  Referenced by SurrogateModel::force_rebuild(), and RecastModel::init_constraints().

**void shape ( )**

shape the lower/upper bound arrays based on sharedVarsData

  Resizes the derived bounds arrays.

  References SharedVariablesData::all_counts(), Constraints::allContinuousLowerBnds, Constraints::allContinuousUpperBnds, Constraints::allDiscreteIntLowerBnds, Constraints::allDiscreteIntUpperBnds, Constraints::allDiscreteRealLowerBnds, Constraints::allDiscreteRealUpperBnds, Constraints::constraintsRep, Constraints::shape(), and Constraints::sharedVarsData.

  Referenced by Constraints::Constraints(), and Constraints::shape().

**void reshape ( size_t num_nln_ineq_cons, size_t num_nln_eq_cons, size_t num_lin_ineq_cons, size_t num_lin_eq_cons )**

reshape the linear/nonlinear constraint arrays

  Resizes the linear and nonlinear constraint arrays at the base class. Does NOT currently resize the derived bounds arrays.

  References Constraints::constraintsRep, Constraints::continuousLowerBnds, Constraints::discreteIntLowerBnds, Constraints::discreteRealLowerBnds, Constraints::linearEqConCoeffs, Constraints::linearEqConTargets, Constraints::linearIneqConCoeffs, Constraints::linearIneqConLowerBnds, Constraints::linearIneqConUpperBnds, Constraints::nonlinearEqConTargets, Constraints::nonlinearEqConCoeffs, Constraints::nonlinearIneqConLowerBnds, Constraints::nonlinearIneqConUpperBnds, Constraints::numLinearEqCons, Constraints::numNonlinearEqCons, Constraints::numNonlinearIneqCons, and Constraints::reshape().
void manage_linear_constraints ( const ProblemDescDB & problem_db ) [protected]

perform checks on user input, convert linear constraint coefficient input to matrices, and assign defaults

Convenience function called from derived class constructors. The number of variables active for applying linear constraints is currently defined to be the number of active continuous variables plus the number of active discrete variables (the most general case), even though very few optimizers can currently support mixed variable linear constraints.

References Dakota::abort_handler(), Constraints::continuousLowerBnds, Dakota::copy_data(), Constraints::discreteIntLowerBnds, Constraints::discreteRealLowerBnds, ProblemDescDB::get_rv(), Constraints::linearEqConCoeffs, Constraints::linearEqConTargets, Constraints::linearIneqConCoeffs, Constraints::linearIneqConLowerBnds, Constraints::linearIneqConUpperBnds, Constraints::numLinearEqCons, and Constraints::numLinearIneqCons.

Referenced by Constraints::Constraints().

Constraints * get_constraints ( const ProblemDescDB & problem_db, const SharedVariablesData & svd ) [private]

Used only by the constructor to initialize constraintsRep to the appropriate derived type.

Initializes constraintsRep to the appropriate derived type, as given by the variables view.

References SharedVariablesData::view().

Referenced by Constraints::Constraints(), and Constraints::copy().

Constraints * get_constraints ( const SharedVariablesData & svd ) const [private]

Used by copy() to initialize constraintsRep to the appropriate derived type.

Initializes constraintsRep to the appropriate derived type, as given by the variables view. The default derived class constructors are invoked.

References SharedVariablesData::view().

The documentation for this class was generated from the following files:

• DakotaConstraints.hpp
• DakotaConstraints.cpp

13.26 DataEnvironment Class Reference

Handle class for environment specification data.

Public Member Functions

• DataEnvironment ()
  constructor

• DataEnvironment (const DataEnvironment &)
  copy constructor

• ~DataEnvironment ()
  destructor

• DataEnvironment & operator= (const DataEnvironment &)
  assignment operator

• void write (std::ostream &s) const
  write a DataEnvironment object to an std::ostream
13.27. DATAENVIRONMENTREP CLASS REFERENCE

• void read (MPIUnpackBuffer &s)
  
  read a DataEnvironment object from a packed MPI buffer

• void write (MPIPackBuffer &s) const
  
  write a DataEnvironment object to a packed MPI buffer

• DataEnvironmentRep * data_rep ()
  
  return dataEnvRep

Private Attributes

• DataEnvironmentRep * dataEnvRep
  
  pointer to the body (handle-body idiom)

Friends

• class ProblemDescDB
• class NIDRProblemDescDB

13.26.1 Detailed Description

Handle class for environment specification data.

The DataEnvironment class is used to provide a memory management handle for the data in DataEnvironment-
Rep. It is populated by IDRProblemDescDB::environment_kwhandler() and is queried by the ProblemDescDB-
::get_<datatype>() functions. A single DataEnvironment object is maintained in ProblemDescDB::environment-
Spec.

The documentation for this class was generated from the following files:

• DataEnvironment.hpp
• DataEnvironment.cpp

13.27 DataEnvironmentRep Class Reference

Body class for environment specification data.

Public Attributes

• bool checkFlag
  
  flag for whether to run in check only mode (default false)

• String outputFile
  
  file name for output redirection (overrides command-line)

• String errorFile
  
  file name for error redirection (overrides command-line)

• String readRestart
  
  file name for restart read (overrides command-line)

• int stopRestart
  
  record at which to stop reading restart

• String writeRestart
file name for restart write (overrides command-line)

- bool preRunFlag
  flags invocation with command line option -pre_run

- bool runFlag
  flags invocation with command line option -run

- bool postRunFlag
  flags invocation with command line option -post_run

- String preRunInput
  filename for pre_run input

- String preRunOutput
  filename for pre_run output

- String runInput
  filename for run input

- String runOutput
  filename for run output

- String postRunInput
  filename for post_run input

- String postRunOutput
  filename for post_run output

- unsigned short preRunOutputFormat
  tabular format for pre_run output

- unsigned short postRunInputFormat
  tabular format for post_run input

- bool graphicsFlag
  flags use of graphics by the environment (from the graphics specification in EnvIndControl)

- bool tabularDataFlag
  flags tabular data collection by the environment (from the tabular_graphics_data specification in EnvIndControl)

- String tabularDataFile
  the filename used for tabular data collection by the environment (from the tabular_graphics_file specification in EnvIndControl)

- unsigned short tabularFormat
  format for tabular data files (see enum)

- int outputPrecision
  output precision for tabular and screen output

- bool resultsOutputFlag
  flags use of results output to default file

- String resultsOutputFile
  named file for results output

- String topMethodPointer
  method identifier for the environment (from the top_method_pointer specification)
13.28. DataFitSurrBasedLocalMinimizer Class Reference

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

Inheritance diagram for DataFitSurrBasedLocalMinimizer:
Public Member Functions

- `DataFitSurrBasedLocalMinimizer (ProblemDescDB &problem_db, Model &model)`
  constructor
- `~DataFitSurrBasedLocalMinimizer ()`
  destructor

Protected Member Functions

- void `pre_run ()`
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void `post_run (std::ostream &s)`
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
- `SurrBasedLevelData & trust_region ()`
  return the active SurrBasedLevelData instance
- void `update_trust_region ()`
  update the trust region bounds, strictly contained within global bounds
- void `build ()`
  build the approximation over the current trust region
- void `minimize ()`
  solve the approximate subproblem
- void `verify ()`
  verify the approximate iterate and update the trust region for the next approximate optimization cycle
- bool `build_global ()`
- bool `build_local ()`
- void `compute_center_correction (bool embed_correction)`
- unsigned short `converged ()`
  return the convergence code for the truth level of the trust region hierarchy
- void `find_center_truth ()`
  retrieve responseCenterTruth if possible, evaluate it if not
- void `find_center_approx ()`
  retrieve responseCenter_approx if possible, evaluate it if not
Protected Attributes

- SurrBasedLevelData trustRegionData
  container for trust region variable/response data
- bool globalApproxFlag
  flags the use of a global data fit surrogate (rsm, ann, mars, kriging)
- bool multiptApproxFlag
  flags the use of a multipoint data fit surrogate (TANA)
- bool localApproxFlag
  flags the use of a local data fit surrogate (Taylor series)
- bool multiLayerBypassFlag
  flags the simultaneous presence of two conditions: (1) additional layerings w/i actual_model (e.g., surrogateModel = layered/nested/layered -> actual_model = nested/layered), and (2) a user-specification to bypass all layerings within actual_model for the evaluation of truth data (responseCenterTruth and responseStarTruth).
- bool useDerivsFlag
  flag for the "use_derivatives" specification for which derivatives are to be evaluated at each DACE point in global surrogate builds.

Additional Inherited Members

13.28.1 Detailed Description

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

This minimizer uses a SurrogateModel to perform minimization based on local, global, or hierarchical surrogates. It achieves provable convergence through the use of a sequence of trust regions and the application of surrogate corrections at the trust region centers.

13.28.2 Member Function Documentation

void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s pre_run(), if implemented, typically before performing its own implementation steps.

Reimplemented from Iterator.

References Response::active_set(), Iterator::active_set(), Model::current_response(), Model::current_variables(), DataFitSurrBasedLocalMinimizer::globalApproxFlag, Iterator::is_null(), Iterator::iteratedModel, SurrBasedLocalMinimizer::origTrustRegionFactor, SurrBasedLocalMinimizer::pre_run(), ActiveSet::request_values(), Model::subordinate_iterator(), DataFitSurrBasedLocalMinimizer::trustRegionData, Model::truth_model(), and DataFitSurrBasedLocalMinimizer::useDerivsFlag.

void post_run ( std::ostream & s ) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s post_run(), typically after performing its own implementation steps.
Reimplemented from Minimizer.

References SurrBasedLocalMinimizer::approxSubProbModel, Iterator::bestResponseArray, Iterator::bestVariablesArray, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), SurrBasedLocalMinimizer::globalLowerBnds, SurrBasedLocalMinimizer::globalUpperBnds, Iterator::iteratedModel, Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, SurrBasedLocalMinimizer::post_run(), SurrBasedLocalMinimizer::recastSubProb, SurrBasedLocalMinimizer::trConstraintRelax, and DataFitSurrBasedLocalMinimizer::trustRegionData.

The documentation for this class was generated from the following files:

- DataFitSurrBasedLocalMinimizer.hpp
- DataFitSurrBasedLocalMinimizer.cpp

### 13.29 DataFitSurrModel Class Reference

Derived model class within the surrogate model branch for managing data fit surrogates (global and local)

Inheritance diagram for DataFitSurrModel:

```
Model
    SurrogateModel
        DataFitSurrModel
```

#### Public Member Functions

- **DataFitSurrModel (ProblemDescDB &problem_db)**
  
  constructor

- **DataFitSurrModel (Iterator &dace_iterator, Model &actual_model, const ActiveSet &set, const String &approx_type, const UShortArray &approx_order, short corr_type, short corr_order, short data_order, short output_level, const String &point_reuse, const String &import_build_points_file=String(), unsigned short import_build_format=TABULAR_ANNOTATED, bool import_build_active_only=false, const String &export_approx_points_file=String(), unsigned short export_approx_format=TABULAR_ANNOTATED)**
  
  alternate constructor for instantiations on the fly

- **~DataFitSurrModel ()**
  
  destructor

- **void total_points (int points)**
  
  set pointsTotal and pointsManagement mode

- **DiscrepancyCorrection & discrepancy_correction ()**
  
  return the DiscrepancyCorrection object used by SurrogateModels
Protected Member Functions

- **bool initialize_mapping** (ParLevLIter pl_iter)
  
  Perform any global updates prior to individual evaluate() calls.

- **bool finalize_mapping** ()
  
  Restore state in preparation for next initialization.

- **void derived_evaluate** (const ActiveSet &set)
  
  Portion of evaluate() specific to DataFitSurrModel.

- **void derived_evaluate_nowait** (const ActiveSet &set)
  
  Portion of evaluate_nowait() specific to DataFitSurrModel.

- **const IntResponseMap & derived_synchronize** ()
  
  Portion of synchronize() specific to DataFitSurrModel.

- **const IntResponseMap & derived_synchronize_nowait** ()
  
  Portion of synchronize_nowait() specific to DataFitSurrModel.

- **Iterator & subordinate_iterator** ()
  
  Return daceIterator.

- **Model & surrogate_model** ()
  
  Return this model instance.

- **Model & truth_model** ()
  
  Return actualModel.

- **void derived_subordinate_models** (ModelList &ml, bool recurse_flag)
  
  Return actualModel (and optionally its sub-models).

- **void update_from_subordinate_model** (size_t depth=std::numeric_limits<size_t>::max())
  
  Pass request to actualModel if recursing and then update from it.

- **Interface & derived_interface** ()
  
  Return approxInterface.

- **void primary_response_fn_weights** (const RealVector &wts, bool recurse_flag=true)
  
  Set the relative weightings for multiple objective functions or least squares terms and optionally recurses into actualModel.

- **void surrogate_response_mode** (short mode)
  
  Set responseMode and pass any bypass request on to actualModel for any lower-level surrogates.

- **void surrogate_function_indices** (const IntSet &surr_fn_indices)
  
  (re)set the surrogate index set in SurrogateModel::surrFnIndices and ApproximationInterface::approxFnIndices.

- **void build_approximation** ()
  
  Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points.

- **bool build_approximation** (const Variables &vars, const IntResponsePair &response_pr)
  
  Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points that augment the passed vars/response anchor point.

- **void update_approximation** (bool rebuild_flag)
  
  Replaces the approximation data with daceIterator results and rebuilds the approximation if requested.

- **void update_approximation** (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)
  
  Replaces the anchor point, and rebuilds the approximation if requested.
void update_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)
   replaces the current points array and rebuilds the approximation if requested

void update_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_flag)
   replaces the current points array and rebuilds the approximation if requested

void append_approximation (bool rebuild_flag)
   appends dacelIterator results to a global approximation and rebuilds it if requested

void append_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)
   appends a point to a global approximation and rebuilds it if requested

void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)
   appends an array of points to a global approximation and rebuilds it if requested

void append_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_flag)
   appends a matrix of points to a global approximation and rebuilds it if requested

void pop_approximation (bool save_surr_data, bool rebuild_flag=false)
   remove approximation data added on previous append_approximation() call or a specified number of points

void push_approximation ()
   retrieve a previous approximation data state

bool push_available ()
   query for whether a trial increment can be retrieved

void finalize_approximation ()
   finalize data fit by applying all previous trial increments

void store_approximation (size_t index=NPOS)
   store the current data fit approximation for later combination

void restore_approximation (size_t index=NPOS)
   restore a previous data fit approximation

void remove_stored_approximation (size_t index=NPOS)
   store the current data fit approximation for later combination

void combine_approximation (short corr_type)
   combine the current data fit approximation with one previously stored

void run_dace_iterator (bool rebuild_flag)
   execute the DACE iterator, append the approximation data, and rebuild the approximation if indicated

SharedApproxData & shared_approximation ()
   retrieve the SharedApproxData from approxInterface

std::vector< Approximation > & approximations ()
   retrieve the set of Approximations from approxInterface

const RealVectorArray & approximation_coefficients (bool normalized=false)
   return the approximation coefficients from each Approximation (request forwarded to approxInterface)

void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)
   set the approximation coefficients within each Approximation (request forwarded to approxInterface)

const RealVector & approximation_variances (const Variables &vars)
return the approximation variance from each Approximation (request forwarded to approxInterface)

- const Pecos::SurrogateData & approximation_data (size_t index)
  return the approximation data from a particular Approximation (request forwarded to approxInterface)

- void component_parallel_mode (short mode)
  update component parallel mode for supporting parallelism in actualModel

- IntIntPair estimate_partition_bounds (int max_eval_concurrency)
  estimate the minimum and maximum partition sizes that can be utilized by this Model

- void derived_init_communicators (ParLevIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  set up actualModel for parallel operations

- void derived_init_serial ()
  set up actualModel for serial operations.

- void derived_set_communicators (ParLevIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  set active parallel configuration within actualModel

- void derived_free_communicators (ParLevIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  deallocate communicator partitions for the DataFitSurrModel (request forwarded to actualModel)

- void serve_run (ParLevIter pl_iter, int max_eval_concurrency)
  Service actualModel job requests received from the master. Completes when a termination message is received from stop_servers().

- void stop_servers ()
  Executed by the master to terminate actualModel server operations when DataFitSurrModel iteration is complete.

- void inactive_view (short view, bool recurse_flag=true)
  update the Model’s inactive view based on higher level (nested) context and optionally recurse into actualModel

- const String & interface_id () const
  return the approxInterface identifier

- bool evaluation_cache (bool recurse_flag=true) const
  if recurse_flag, return the actualModel evaluation cache usage

- bool restart_file (bool recurse_flag=true) const
  if recurse_flag, return the actualModel restart file usage

- void set_evaluation_reference ()
  set the evaluation counter reference points for the DataFitSurrModel (request forwarded to approxInterface and actualModel)

- void fine_grained_evaluation_counts ()
  request fine-grained evaluation reporting within approxInterface and actualModel

- void print_evaluation_summary (std::ostream &, bool minimal_header=false, bool relative_count=true) const
  print the evaluation summary for the DataFitSurrModel (request forwarded to approxInterface and actualModel)

- void warm_start_flag (const bool flag)
  set the warm start flag, including actualModel
Protected Attributes

- const bool exportSurrogate
  whether to export the surrogate to file
- const bool autoRefine
  whether to automatically refine the surrogate during the build phase
- const int maxIterations
  Maximum number of times to refine the surrogate.
- const int maxFuncEvals
  Maximum number of evaluations while refining a surrogate.
- const Real convergenceTolerance
  Convergence criterion, compared to CV score for specified metric.
- const int softConvergenceLimit
  Max number of iterations for which there is no average improvement.
- const String refineCVMetric
  Type of error metric to test for surrogate refinement convergence.
- const int refineCVFolds
  Number of cross validation folds for surrogate refinement.

Private Member Functions

- void import_points (unsigned short tabular_format, bool active_only)
  optionally read surrogate data points from provided file
- void initialize_export ()
  initialize file stream for exporting surrogate evaluations
- void finalize_export ()
  finalize file stream for exporting surrogate evaluations
- void export_point (int eval_id, const Variables &vars, const Response &resp)
  initialize file stream for exporting surrogate evaluations
- void derived_synchronize_approx (bool block, IntResponseMap &approx_resp_map_rekey)
  Common code for processing of approximate response maps shared by derived_synchronize() and derived_synchronize_nowait()
- void update_global ()
  Updates fit arrays for global approximations.
- void update_local_multipoint ()
  Updates fit arrays for local or multipoint approximations.
- void build_global ()
  Builds a global approximation using daceIterator.
- void build_local_multipoint ()
  Builds a local or multipoint approximation using actualModel.
- void refine_surrogate ()
  Refine the built surrogate until convergence criteria are met.
- void interface_build_approx ()
  Call build_approximation on the interface, passing appropriate constraints.
• void init_model (Model &model)
  update actualModel with data from constraints/labels/sets
• void update_model (Model &model)
  update actualModel with data from current variables/bounds
• void update_from_model (const Model &model)
  update current variables/labels/bounds/targets with data from actualModel
• bool vars_exact_compare (const Variables &vars, const Pecos::SurrogateDataVars &sdv) const
  test for exact equality in values between vars and sdv
• bool inside (const RealVector &c_vars, const IntVector &di_vars, const RealVector &dr_vars) const
  test if c_vars and d_vars are within [c_l_bnds,c_u_bnds] and [d_l_bnds,d_u_bnds]

Private Attributes

• DiscrepancyCorrection deltaCorr
  manages construction and application of correction functions that are applied to a surrogate model (DataFitSurr
  or HierarchSurr) in order to reproduce high fidelity data.
• int pointsTotal
  total points the user specified to construct the surrogate
• short pointsManagement
  configuration for points management in build_global()
• String pointReuse
  type of point reuse for approximation builds: all, region (default if points file), or none (default if no points
  file)
• String importPointsFile
  file name from import_build_points_file specification
• String exportPointsFile
  file name from export_approx_points_file specification
• unsigned short exportFormat
  file export format for variables and approximate responses
• std::ofstream exportFileStream
  output file stream for export_approx_points_file specification
• Interface approxInterface
  manages the building and subsequent evaluation of the approximations (required for both global and local)
• Model actualModel
  the truth model which provides evaluations for building the surrogate (optional for global, required for local)
• Iterator daceIterator
  selects parameter sets on which to evaluate actualModel in order to generate the necessary data for building global
  approximations (optional for global since restart data may also be used)
Additional Inherited Members

13.29.1 Detailed Description

Derived model class within the surrogate model branch for managing data fit surrogates (global and local)

The DataFitSurrModel class manages global or local approximations (surrogates that involve data fits) that are
used in place of an expensive model. The class contains an approxInterface (required for both global and local)
which manages the approximate function evaluations, an actualModel (optional for global, required for local)
which provides truth evaluations for building the surrogate, and a daceIterator (optional for global, not used for
local) which selects parameter sets on which to evaluate actualModel in order to generate the necessary data for
building global approximations.

13.29.2 Constructor & Destructor Documentation

\[\sim\text{DataFitSurrModel()}\] [inline]

destructor

Virtual destructor handles referenceCount at base Model level.
References DataFitSurrModel::finalize_export().

13.29.3 Member Function Documentation

\text{bool finalize_mapping()} [protected], [virtual]

restore state in preparation for next initialization

Inactive variables must be propagated when a HierarchSurrModel is employed by a sub-iterator (e.g., OUU
with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::
initialize_mapping().

Reimplemented from Model.
References DataFitSurrModel::actualModel, SurrogateModel::finalize_mapping(), and Model::finalize_mapping().

\text{void derived_evaluate ( const ActiveSet & set )} [protected], [virtual]

portion of evaluate() specific to DataFitSurrModel

Compute the response synchronously using actualModel, approxInterface, or both (mixed case). For the
approxInterface portion, build the approximation if needed, evaluate the approximate response, and apply correc-
tion (if active) to the results.

Reimplemented from Model.
References Response::active_set(), DataFitSurrModel::actualModel, DiscrepancyCorrection::apply(), Surrogate-
Model::approxBuilds, DataFitSurrModel::approxInterface, SurrogateModel::asv_mapping(), DataFitSurrModel::
build_approximation(), DataFitSurrModel::component_parallel_mode(), DiscrepancyCorrection::compute(), Response-
copy(), Model::current_response(), Model::currentResponse, Model::currentVariables, DataFitSurrModel::delta-
Corr, Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate(), DataFitSurrModel::export_point(), Surrogate-
Model::force_rebuild(), Model::hierarchicalTagging, Interface::map(), Model::outputLevel, ActiveSet::request-
vector(), SurrogateModel::response_mapping(), SurrogateModel::responseMode, SurrogateModel::surrModelEval-
Cntr, Response::update(), and DataFitSurrModel::update_model().

\text{void derived_evaluate_nowait ( const ActiveSet & set )} [protected], [virtual]

portion of evaluate_nowait() specific to DataFitSurrModel
Compute the response asynchronously using actualModel, approxInterface, or both (mixed case). For the approxInterface portion, build the approximation if needed and evaluate the approximate response in a quasi-asynchronous approach (ApproximationInterface::map() performs the map synchronously and bookkeeps the results for return in derived::synchronize() below).

Reimplemented from Model.

References DataFitSurrModel::actualModel, SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, SurrogateModel::asv_mapping(), DataFitSurrModel::build_approximation(), Variables::copy(), Model::currentResponse, Model::currentVariables, Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate_nowait(), Interface::evaluation_id(), Model::evaluation_id(), DataFitSurrModel::exportPointsFile, SurrogateModel::force_rebuild(), Model::hierarchical-Tagging, Interface::map(), SurrogateModel::rawVarsMap, ActiveSet::request_vector(), SurrogateModel::response-Mode, SurrogateModel::surrIdMap, SurrogateModel::surrModelEvalCntr, SurrogateModel::truthIdMap, and DataFitSurrModel::update_model().

const IntResponseMap & derived_synchronize ( ) [protected], [virtual]

portion of synchronize() specific to DataFitSurrModel

Blocking retrieval of asynchronous evaluations from actualModel, approxInterface, or both (mixed case). For the approxInterface portion, apply correction (if active) to each response in the array. derived::synchronize() is designed for the general case where derived::evaluate_nowait() may be inconsistent in its use of actual evaluations, approximate evaluations, or both.

Reimplemented from Model.

References DataFitSurrModel::actualModel, SurrogateModel::aggregate_response(), SurrogateModel::check_key(), DataFitSurrModel::component_parallel_mode(), DiscrepancyCorrection::compute(), DataFitSurrModel::delta-Corr, DataFitSurrModel::derived_synchronize_approx(), Model::outputLevel, Model::rekey_synch(), SurrogateModel::response_mapping(), SurrogateModel::responseMode, SurrogateModel::surrIdMap, SurrogateModel::surrResponseMap, and SurrogateModel::truthIdMap.

const IntResponseMap & derived_synchronize_nowait ( ) [protected], [virtual]

portion of synchronize_nowait() specific to DataFitSurrModel

Nonblocking retrieval of asynchronous evaluations from actualModel, approxInterface, or both (mixed case). For the approxInterface portion, apply correction (if active) to each response in the map. derived::synchronize_nowait() is designed for the general case where derived::evaluate_nowait() may be inconsistent in its use of actual evals, approx evals, or both.

Reimplemented from Model.

References Dakota::abort_handler(), DataFitSurrModel::actualModel, SurrogateModel::aggregate_response(), SurrogateModel::cachedApproxRespMap, DataFitSurrModel::component_parallel_mode(), DiscrepancyCorrection::compute(), DataFitSurrModel::deltaCorr, DataFitSurrModel::derived_synchronize_approx(), Model::outputLevel, Model::rekey_synch(), SurrogateModel::response_mapping(), SurrogateModel::responseMode, SurrogateModel::surrIdMap, SurrogateModel::surrResponseMap, and SurrogateModel::truthIdMap.

void build_approximation ( ) [protected], [virtual]

Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points.

This function constructs a new approximation, discarding any previous data. It constructs any required data for SurrogateData::{vars,resp}Data and does not define an anchor point for SurrogateData::anchor{Vars,Resp}, so is an unconstrained build.

Reimplemented from Model.
References DataFitSurrModel::actualModel, SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, DataFitSurrModel::autoRefine, DataFitSurrModel::build_global, DataFitSurrModel::build_local_multipoint, Interface::clear_current, DataFitSurrModel::interface_build_approx, DataFitSurrModel::refine_surrogate, Dakota::strbegins, Model::surrogateType, DataFitSurrModel::update_global, DataFitSurrModel::update_local_multipoint, and DataFitSurrModel::update_model.

Referenced by DataFitSurrModel::derived_evaluate, and DataFitSurrModel::derived_evaluate_nowait.

```cpp
bool build_approximation ( const Variables & vars, const IntResponsePair & response )
protected, virtual
```

Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points that augment the passed vars/response anchor point.

This function constructs a new approximation, discarding any previous data. It uses the passed data to populate SurrogateData::anchor{Vars,Resp} and constructs any required data points for SurrogateData::{vars,resp}Data.

Reimplemented from Model.

References DataFitSurrModel::actualModel, SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, DataFitSurrModel::autoRefine, DataFitSurrModel::build_global, Interface::clear_current, DataFitSurrModel::interface_build_approx, DataFitSurrModel::refine_surrogate, Dakota::strbegins, Model::surrogateType, Interface::update_approximation, DataFitSurrModel::update_global, DataFitSurrModel::update_local_multipoint, and DataFitSurrModel::update_model.

```cpp
void update_approximation ( bool rebuild_flag )
protected, virtual
```

replaces the approximation data with daceIterator results and rebuilds the approximation if requested.

This function populates/replaces SurrogateData::anchor{Vars,Resp} and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::{vars,resp}Data) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Iterator::all_responses, Iterator::all_samples, Iterator::all_variables, SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, Iterator::compact_mode, DataFitSurrModel::daceIterator, Model::numFns, Model::outputLevel, Interface::rebuild_approximation, Model::surrogateType, and Interface::update_approximation.

```cpp
void update_approximation ( const Variables & vars, const IntResponsePair & response, bool rebuild_flag )
protected, virtual
```

replaces the anchor point, and rebuilds the approximation if requested.

This function populates/replaces SurrogateData::anchor{Vars,Resp} and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::{vars,resp}Data) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, Model::numFns, Model::outputLevel, Interface::rebuild_approximation, Model::surrogateType, and Interface::update_approximation.

```cpp
void update_approximation ( const VariablesArray & vars_array, const IntResponseMap & resp_map, bool rebuild_flag )
protected, virtual
```

replaces the current points array and rebuilds the approximation if requested.
This function populates/replaces SurrogateData::\{vars,resp\}Data and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::anchor\{Vars,Resp\}) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build\_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, Model::numFns, Model::outputLevel, Interface::rebuild\_approximation(), Model::surrogateType, and Interface::update\_approximation().

```cpp
void update\_approximation ( const RealMatrix & samples, const IntResponseMap & resp\_map, bool rebuild\_flag ) [protected], [virtual]
```
replaces the current points array and rebuilds the approximation if requested

This function populates/replaces SurrogateData::\{vars,resp\}Data and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::anchor\{Vars,Resp\}) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build\_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, Model::numFns, Model::outputLevel, Interface::rebuild\_approximation(), Model::surrogateType, and Interface::update\_approximation().

```cpp
void append\_approximation ( bool rebuild\_flag ) [protected], [virtual]
```
appends daceIterator results to a global approximation and rebuilds it if requested

This function appends one point to SurrogateData::\{vars,resp\}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor\{Vars,Resp\}) and does not update the actualModel with revised bounds, labels, etc. Thus, it appends to data from a previous call to build\_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Iterator::all\_responses(), Iterator::all\_samples(), Iterator::all\_variables(), Interface::append\_approximation(), SurrogateModel::approxBuilds, DataFitSurrModel::approx\_Interface, Iterator::compact\_mode(), DataFitSurrModel::daceIterator, Model::numFns, Model::output\_Level, Interface::rebuild\_approximation(), and Model::surrogate\_Type.

Referenced by DataFitSurrModel::run\_dace\_iterator().

```cpp
void append\_approximation ( const Variables & vars, const IntResponsePair & response\_pr, bool rebuild\_flag ) [protected], [virtual]
```
appends a point to a global approximation and rebuilds it if requested

This function appends one point to SurrogateData::\{vars,resp\}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor\{Vars,Resp\}) and does not update the actualModel with revised bounds, labels, etc. Thus, it appends to data from a previous call to build\_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Interface::append\_approximation(), SurrogateModel::approxBuilds, DataFitSurrModel::approx\_Interface, Model::numFns, Model::output\_Level, Interface::rebuild\_approximation(), and Model::surrogate\_Type.

```cpp
void append\_approximation ( const VariablesArray & vars\_array, const IntResponseMap & resp\_map, bool rebuild\_flag ) [protected], [virtual]
```
appends an array of points to a global approximation and rebuilds it if requested
This function appends multiple points to SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actual-Model with revised bounds, labels, etc. Thus, it appends to data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Interface::append_approximation(), SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, Model::numFns, Model::outputLevel, Interface::rebuild_approximation(), and Model::surrogateType.

```cpp
void append_approximation ( const RealMatrix & samples, const IntResponseMap & resp_map, bool rebuild_flag ) [protected], [virtual]
```

appends a matrix of points to a global approximation and rebuilds it if requested

This function appends multiple points to SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actual-Model with revised bounds, labels, etc. Thus, it appends to data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Interface::append_approximation(), SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, Model::numFns, Model::outputLevel, Interface::rebuild_approximation(), and Model::surrogateType.

```cpp
void derived_init_communicators ( ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag = true ) [protected], [virtual]
```

set up actualModel for parallel operations

asynchronous flags need to be initialized for the sub-models. In addition, max_eval_concurrency is the outer level iterator concurrency, not the DACE concurrency that actualModel will see, and recomputing the message-lengths on the sub-model is probably not a bad idea either. Therefore, recompute everything on actualModel using init_communicators.

Reimplemented from Model.

References DataFitSurrModel::actualModel, DataFitSurrModel::approxInterface, DataFitSurrModel::daceIterator, Model::derivative_concurrency(), ProblemDescDB::get_db_method_node(), ProblemDescDB::get_db_model_node(), Iterator::init_communicators(), Model::init_communicators(), Iterator::is_null(), Model::is_null(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_id(), Interface::minimum_points(), Model::model_id(), Model::probDescDB, ProblemDescDB::set_db_list_nodes(), ProblemDescDB::set_db_method_node(), and ProblemDescDB::set_db_model_nodes().

```cpp
void import_points ( unsigned short tabular_format, bool active_only ) [private]
```

optionally read surrogate data points from provided file

Constructor helper to read the points file once, if provided, and then reuse its data as appropriate within build_global(). Surrogate data imports default to active/inactive variables, but user can override to active only process arrays of data from TabularIO::read_data_tabular() above

References DataFitSurrModel::actualModel, Model::current_response(), Model::current_variables(), Model::currentResponse, Model::currentVariables, Variables::cv(), Dakota::data_pairs, Variables::div(), Variables::drv(), Variables::dsv(), ParamResponsePair::eval_id(), Model::evaluation_cache(), DataFitSurrModel::importPointsFile, ParamResponsePair::interface_id(), Model::interface_id(), Model::is_null(), Model::numFns, Model::outputLevel, Model::parallelLib, Model::restart_file(), Variables::tv(), and ParallelLibrary::write_restart().

Referenced by DataFitSurrModel::DataFitSurrModel().
void initialize_export() [private]
initialize file stream for exporting surrogate evaluations

Constructor helper to export approximation-based evaluations to a file.
References Model::currentResponse, Model::currentVariables, DataFitSurrModel::exportFileStream, DataFitSurrModel::exportFormat, and DataFitSurrModel::exportPointsFile.
Referenced by DataFitSurrModel::DataFitSurrModel().

void finalize_export() [private]
finalize file stream for exporting surrogate evaluations

Constructor helper to export approximation-based evaluations to a file.
References DataFitSurrModel::exportFileStream, and DataFitSurrModel::exportPointsFile.
Referenced by DataFitSurrModel::DataFitSurrModel().

void export_point(int eval_id, const Variables & vars, const Response & resp) [private]
initialize file stream for exporting surrogate evaluations

Constructor helper to export approximation-based evaluations to a file. Exports all variables, so it’s clear at what values of inactive it was built at
References DataFitSurrModel::exportFileStream, DataFitSurrModel::exportFormat, DataFitSurrModel::exportPointsFile, DataFitSurrModel::interface_id(), Model::iterator_space_to_user_space(), and Model::recastings().
Referenced by DataFitSurrModel::derived_evaluate(), and DataFitSurrModel::derived_synchronize_approx().

void build_global() [private]
Builds a global approximation using daceIterator.

Determine points to use in building the approximation and then evaluate them on actualModel using daceIterator. Any changes to the bounds should be performed by setting them at a higher level (e.g., SurrogateOptStrategy).
References Dakota::abort_handler(), DataFitSurrModel::actualModel, Interface::append_approximation(), Interface::approximation_data(), DataFitSurrModel::approxInterface, DataFitSurrModel::component_parallel_mode(), Variables::continuous_variables(), Model::currentVariables, Variables::cv(), Model::cv(), DataFitSurrModel::daceIterator, Dakota::data_pairs, Variables::discrete_int_variables(), Variables::discrete_real_variables(), Variables::div(), Model::div(), Variables::drv(), Model::drv(), DataFitSurrModel::inside(), Model::interface_id(), Iterator::is_null(), Model::is_null(), Interface::minimum_points(), Iterator::num_samples(), Model::outputLevel, DataFitSurrModel::point_Reuse, DataFitSurrModel::pointsManagement, DataFitSurrModel::pointsTotal, Model::recastings(), Interface::recommended_points(), DataFitSurrModel::run_dace_iterator(), Iterator::sampling_reset(), SurrogateModel::surrogateFnIndices, Model::user_space_to_iterator_space(), and DataFitSurrModel::vars_exact_compare().
Referenced by DataFitSurrModel::build_approximation().

void build_local_multipoint() [private]
Builds a local or multipoint approximation using actualModel.

Evaluate the value, gradient, and possibly Hessian needed for a local or multipoint approximation using actualModel.
References Response::active_set(), DataFitSurrModel::actualModel, DataFitSurrModel::approxInterface, SurrogateModel::asv_mapping(), DataFitSurrModel::component_parallel_mode(), Model::continuous_variable_ids(), Model::current_response(), Model::current_variables(), ActiveSet::derivative_vector(), Model::evaluate(), Model::evaluation_id(), Model::hessian_type(), Model::numFns, ActiveSet::request_vector(), Dakota::strbegins(), Model::surrogate-Type, and Interface::update_approximation().
void init_model ( Model & model )  [private]

update actualModel with data from constraints/labels/sets

Update variables and constraints data within model using values and labels from currentVariables and bound/linear/nonlinear constraints from userDefinedConstraints.

References Dakota::abort_handler(), Model::aleatDistParams, Model::aleatory_distribution_parameters(), Variables::all_continuous_variable_labels(), Model::all_continuous_variable_labels(), Variables::all_discrete_int_variable_labels(), Model::all_discrete_int_variable_labels(), Variables::all_discrete_real_variable_labels(), Model::all_discrete_real_variable_labels(), SurrogateModel::approxBuilds, Variables::continuous_variable_labels(), Model::continuous_variable_labels(), Model::current_variables(), Model::currentResponse, Model::currentVariables, Variables::cv(), Model::cv(), Model::discrete_design_set_int_values(), Model::discrete_design_set_real_values(), Variables::discrete_int_variable_labels(), Model::discrete_int_variable_labels(), Variables::discrete_real_variable_labels(), Model::discrete_real_variable_labels(), Model::discrete_state_set_int_values(), Model::discrete_state_set_real_values(), Model::discrete_designSetIntValues, Model::discreteDesignSetRealValues, Constraints::linearconstraint_coeffs(), Model::linearconstraint_coeffs(), Constraints::linear_constraint_coeffs(), Model::linear_constraint_coeffs(), Constraints::linear_constraint_lower_bounds(), Model::linear_constraint_lower_bounds(), Constraints::linear_constraint_upper_bounds(), Model::linear_constraint_upper_bounds(), Constraints::nonlinear_eq_constraint_coeffs(), Model::nonlinear_eq_constraint_coeffs(), Constraints::nonlinear_eq_constraint_lower_bounds(), Model::nonlinear_eq_constraint_lower_bounds(), Constraints::nonlinear_eq_constraint_upper_bounds(), Model::nonlinear_eq_constraint_upper_bounds(), Constraints::num_linear_eq_constraints(), Constraints::num_linear_ineq_constraints(), Constraints::num_nonlinear_eq_constraints(), Constraints::num_nonlinear_ineq_constraints(), Model::response_labels(), Variables::shared_data(), Model::userDefinedConstraints, and Variables::view().

Referenced by DataFitSurrModel::initialize_mapping().

void update_model ( Model & model )  [private]

update actualModel with data from current variables/bounds

Update variables and constraints data within model using values and labels from currentVariables and bound/linear/nonlinear constraints from userDefinedConstraints.

References Dakota::abort_handler(), Constraints::all_continuous_lower_bounds(), Model::all_continuous_lower_bounds(), Constraints::all_continuous_upper_bounds(), Model::all_continuous_upper_bounds(), Variables::all_continuous_variable_labels(), Model::all_continuous_variable_labels(), Constraints::all_discrete_int_lower_bounds(), Model::all_discrete_int_lower_bounds(), Constraints::all_discrete_int_upper_bounds(), Model::all_discrete_int_upper_bounds(), Variables::all_discrete_int_variable_labels(), Model::all_discrete_int_variable_labels(), Constraints::all_discrete_real_lower_bounds(), Model::all_discrete_real_lower_bounds(), Constraints::all_discrete_real_upper_bounds(), Model::all_discrete_real_upper_bounds(), Variables::all_discrete_real_variable_labels(), Model::all_discrete_real_variable_labels(), Constraints::continuous_lower_bounds(), Model::continuous_lower_bounds(), Constraints::continuous_upper_bounds(), Model::continuous_upper_bounds(), Variables::continuous_variable_labels(), Model::continuous_variable_labels(), Model::currentVariables, Constraints::discrete_lower_bounds(), Model::discrete_lower_bounds(), Constraints::discrete_upper_bounds(), Model::discrete_upper_bounds(), Variables::discrete_variable_labels(), Model::discrete_variable_labels(), Constraints::discrete_int_lower_bounds(), Model::discrete_int_lower_bounds(), Constraints::discrete_int_upper_bounds(), Model::discrete_int_upper_bounds(), Variables::discrete_int_variable_labels(), Model::discrete_int_variable_labels(), Constraints::discrete_real_lower_bounds(), Model::discrete_real_lower_bounds(), Constraints::discrete-
13.29. DATAFITSURRMODEL CLASS REFERENCE

void update_from_model ( const Model & model ) [private]

update current variables/labels/bounds/targets with data from actualModel

Update values and labels in currentVariables and bound/linear/nonlinear constraints in userDefinedConstraints from variables and constraints data within model.

References Dakota::abort_handler(), Model::aleatDistParams, Model::aleatory_distribution_parameters(), Constraints::all_continuous_lower_bounds(), Model::all_continuous_upper_bounds(), Variables::all_continuous_labels(), Model::all_continuous_variable_labels(), Variables::all_continuous_variables(), Constraints::all_discrete_int_lower_bounds(), Model::all_discrete_int_upper_bounds(), Variables::all_discrete_int_variable_labels(), Model::all_discrete_int_variables(), Variables::all_discrete_int_variable_labels(), Model::all_discrete_int_variables(), Variables::all_discrete_int_variable_labels(), Model::all_discrete_int_variables(), Variables::all_discrete_real_labels(), Model::all_discrete_real_variable_labels(), Variables::all_discrete_real_variables(), Constraints::all_discrete_real_lower_bounds(), Model::all_discrete_real_upper_bounds(), Variables::all_discrete_real_variable_labels(), Model::all_discrete_real_variable_labels(), Variables::all_discrete_real_variables(), Model::all_discrete_real_variable_labels(), Variables::all_discrete_real_variables(), SurrogateModel::approxBuilds, Model::current_variables(), Model::currentResponse, Model::currentVariables, Variables::cv(), Model::cv(), Model::discrete_design_set_int_values(), Model::discrete_design_set_real_values(), Model::discrete_state_set_int_values(), Model::discreteDesignSetIntValues, Model::discreteDesignSetRealValues, Model::discreteStateSetIntValues, Model::discreteStateSetRealValues, Variables::div(), Model::div(), Variables::drv(), Model::drv(), Model::epistDistParams, Model::epistemic_distribution_parameters(), Response::function_labels(), SharedVariablesData::id(), Constraints::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_coeffs(), Constraints::linear_eq_constraint_targets(), Model::linear_eq_constraint_targets(), Constraints::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_coeffs(), Constraints::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_lower_bounds(), Constraints::linear_ineq_constraint_upper_bounds(), Model::linear_ineq_constraint_upper_bounds(), Constraints::nonlinear_eq_constraint_targets(), Model::nonlinear_eq_constraint_targets(), Constraints::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_lower_bounds(), Constraints::nonlinear_ineq_constraint_upper_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Constraints::nonlinear_ineq_constrainsto_ineq_constraints(), Model::nonlinear_ineq_constrainsto_ineq_constraints(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Model::primaryRespFnSensSes, Model::primaryRespFnWts, Model::response_labels(), Variables::shared_data(), and Model::userDefinedConstraints.

Referenced by DataFitSurrModel::DataFitSurrModel(), and DataFitSurrModel::update_from_subordinate_model().

13.29.4 Member Data Documentation

Model actualModel [private]

the truth model which provides evaluations for building the surrogate (optional for global, required for local)

actualModel is unrestricted in type; arbitrary nestings are possible.

Referenced by DataFitSurrModel::build_approximation(), DataFitSurrModel::build_global(), DataFitSurrModel::build_local_multipoint(), DataFitSurrModel::DataFitSurrModel(), DataFitSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate_nowait(), DataFitSurrModel::derived_free_communicators(), DataFitSurrModel::derived_init_communicators(), DataFitSurrModel::derived_init_serial(), DataFitSurrModel::derived_set_communicators(), DataFitSurrModel::derived_subordinate_models(), DataFitSurrModel::derived_synchronize(), DataFitSurrModel::derived_synchronize_nowait(), DataFitSurrModel::estimate_partition_bounds(), DataFitSurrModel::evaluation_cache(), DataFitSurrModel::finalize_mapping(), DataFitSurrModel::fine_grained_evaluation_counts(), DataFit-
SurrModel::import_points(), DataFitSurrModel::inactive_view(), DataFitSurrModel::initialize_mapping(), DataFitSurrModel::inside(), DataFitSurrModel::interface_build_approx(), DataFitSurrModel::primary_response_fn_weights(), DataFitSurrModel::print_evaluation_summary(), DataFitSurrModel::restart_file(), DataFitSurrModel::serve_run(), DataFitSurrModel::stop_servers(), DataFitSurrModel::surrogate_response_mode(), DataFitSurrModel::truth_model(), DataFitSurrModel::update_from_subordinate_model(), DataFitSurrModel::update_global(), DataFitSurrModel::update_local_multipoint(), and DataFitSurrModel::warm_start_flag.

The documentation for this class was generated from the following files:

- DataFitSurrModel.hpp
- DataFitSurrModel.cpp

### 13.30 DataInterface Class Reference

Handle class for interface specification data.

**Public Member Functions**

- **DataInterface ()**  
  *constructor*
- **DataInterface (const DataInterface &)**  
  *copy constructor*
- **~DataInterface ()**  
  *destructor*
- **DataInterface & operator= (const DataInterface &)**  
  *assignment operator*
- **void write (std::ostream &s) const**  
  *write a DataInterface object to an std::ostream*
- **void read (MPIUnpackBuffer &s)**  
  *read a DataInterface object from a packed MPI buffer*
- **void write (MPIPackBuffer &s) const**  
  *write a DataInterface object to a packed MPI buffer*
- **DataInterfaceRep * data_rep ()**  
  *return dataIfaceRep*

**Static Public Member Functions**

- **static bool id_compare (const DataInterface &di, const std::string &id)**  
  *compares the idInterface attribute of DataInterface objects*

**Private Attributes**

- **DataInterfaceRep * datafaceRep**  
  *pointer to the body (handle-body idiom)*
13.31. DATAMETHOD CLASS REFERENCE

Friends
- class ProblemDescDB
- class NIDRProblemDescDB

13.30.1 Detailed Description
Handle class for interface specification data.

The DataInterface class is used to provide a memory management handle for the data in DataInterface-Rep. It is populated by IDRProblemDescDB::interface_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataInterface objects is maintained in ProblemDescDB::dataInterfaceList, one for each interface specification in an input file.

The documentation for this class was generated from the following files:
- DataInterface.hpp
- DataInterface.cpp

13.31 DataMethod Class Reference
Handle class for method specification data.

Public Member Functions
- DataMethod ()
  constructor
- DataMethod (const DataMethod &)
  copy constructor
- ~DataMethod ()
  destructor
- DataMethod & operator= (const DataMethod &)
  assignment operator
- void write (std::ostream &s) const
  write a DataMethod object to an std::ostream
- void read (MPIUnpackBuffer &s)
  read a DataMethod object from a packed MPI buffer
- void write (MPIPackBuffer &s) const
  write a DataMethod object to a packed MPI buffer
- DataMethodRep * data_rep ()
  return dataMethodRep

Static Public Member Functions
- static bool id_compare (const DataMethod &dm, const std::string &id)
  compares the idMethod attribute of DataMethod objects
Private Attributes

- DataMethodRep * dataMethodRep
  pointer to the body (handle-body idiom)

Friends

- class ProblemDescDB
- class NIDRProblemDescDB

13.31.1 Detailed Description

Handle class for method specification data.

The DataMethod class is used to provide a memory management handle for the data in DataMethodRep. It is populated by IDRProblemDescDB::method_khandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataMethod objects is maintained in ProblemDescDB::dataMethodList, one for each method specification in an input file.

The documentation for this class was generated from the following files:

- DataMethod.hpp
- DataMethod.cpp

13.32 DataMethodRep Class Reference

Body class for method specification data.

Public Attributes

- String idMethod
  string identifier for the method specification data set (from the id_method specification in MethodIndControl)
- String modelPointer
  string pointer to the model specification to be used by this method (from the model_pointer specification in MethodIndControl)
- String lowFidModelPointer
  string to point to the low fidelity model for Bayesian experimental design
- short methodOutput
  method verbosity control: [SILENT,QUIET,NORMAL,VERBOSE,DEBUG].OUTPUT (from the output specification in MethodIndControl)
- int maxIterations
  maximum number of iterations allowed for the method (from the max_iterations specification in MethodIndControl)
- int maxRefineIterations
  maximum number of refinement iterations allowed for a uniform/adaptive refinement approach (from the max_re refinement_iterations specification in MethodIndControl)
- int maxSolverIterations
  maximum number of internal solver iterations allowed for the method (from the max_solver_iterations specification in MethodIndControl)
- int maxFunctionEvaluations
maximum number of function evaluations allowed for the method (from the \texttt{max\_function\_evaluations} specification in \texttt{MethodIndControl})

- \texttt{bool speculativeFlag}
  flag for use of speculative gradient approaches for maintaining parallel load balance during the line search portion of optimization algorithms (from the \texttt{speculative} specification in \texttt{MethodIndControl})

- \texttt{bool methodUseDerivsFlag}
  flag for usage of derivative data to enhance the computation of surrogate models (PCE/SC expansions, GP models for EGO/EGRA/EGIE) based on the \texttt{use\_derivatives} specification

- \texttt{Real convergenceTolerance}
  iteration convergence tolerance for the method (from the \texttt{convergence\_tolerance} specification in \texttt{MethodIndControl})

- \texttt{Real constraintTolerance}
  tolerance for controlling the amount of infeasibility that is allowed before an active constraint is considered to be violated (from the \texttt{constraint\_tolerance} specification in \texttt{MethodIndControl})

- \texttt{bool methodScaling}
  flag indicating scaling status (from the \texttt{scaling} specification in \texttt{MethodIndControl})

- \texttt{size\_t numFinalSolutions}
  number of final solutions returned from the iterator

- \texttt{unsigned short methodName}
  the method selection: one of the optimizer, least squares, nond, dace, or parameter study methods

- \texttt{unsigned short subMethod}
  enum value for a sub-method type

- \texttt{String subMethodName}
  string identifier for a sub-method name within a multi-option method specification (e.g., from meta-iterators)

- \texttt{String subModelPointer}
  string pointer for a sub-model specification used by a meta-iterator

- \texttt{String subMethodPointer}
  string pointer for a sub-method specification used by a meta-iterator

- \texttt{int iteratorServers}
  number of servers for concurrent iterator parallelism (from the \texttt{iterator\_servers} specification)

- \texttt{int procsPerIterator}
  number of processors for each concurrent iterator partition (from the \texttt{processors\_per\_iterator} specification)

- \texttt{short iteratorScheduling}
  type of scheduling (\{DEFAULT,MASTER,PEER\\_SCHEDULING\}) used in concurrent iterator parallelism (from the \texttt{iterator\_scheduling} specification)

- \texttt{StringArray hybridMethodNames}
  array of methods for the sequential and collaborative hybrid meta-iterators (from the \texttt{method\_name\_list} specification)

- \texttt{StringArray hybridModelPointers}
  array of models for the sequential and collaborative hybrid meta-iterators (from the \texttt{model\_pointer\_list} specification)

- \texttt{StringArray hybridMethodPointers}
  array of methods for the sequential and collaborative hybrid meta-iterators (from the \texttt{method\_pointer\_list} specification)
- **String** `hybridGlobalMethodName`  
  global method name for embedded hybrids (from the `global_method_name` specification)

- **String** `hybridGlobalModelPointer`  
  global model pointer for embedded hybrids (from the `global_model_pointer` specification)

- **String** `hybridGlobalMethodPointer`  
  global method pointer for embedded hybrids (from the `global_method_pointer` specification)

- **String** `hybridLocalMethodName`  
  local method name for embedded hybrids (from the `local_method_name` specification)

- **String** `hybridLocalModelPointer`  
  local model pointer for embedded hybrids (from the `local_model_pointer` specification)

- **String** `hybridLocalMethodPointer`  
  local method pointer for embedded hybrids (from the `local_method_pointer` specification)

- **Real** `hybridLSProb`  
  local search probability for embedded hybrids (from the `local_search_probability` specification)

- **int** `concurrentRandomJobs`  
  number of random jobs to perform in the pareto set and multi_start meta-iterators (from the `random_starts` and `random_weight_sets` specifications)

- **RealVector** `concurrentParameterSets`  
  user-specified (i.e., nonrandom) parameter sets to evaluate in the pareto set and multi_start meta-iterators (from the `starting_points` and `weight_sets` specifications)

- **unsigned short** `softConvLimit`  
  number of consecutive iterations with change less than convergenceTolerance required to trigger convergence

- **bool** `surrBasedLocalLayerBypass`  
  flag to indicate user-specification of a bypass of any/all layerings in evaluating truth response values in SBL.

- **RealVector** `trustRegionInitSize`  
  initial trust region sizes in the surrogate-based local method (from the `initial_size` specification in MethodSBL), one size per surrogate model (notes: no trust region for the truth model; sizes are relative values, e.g., 0.1 = 10% of range of global bounds for each variable)

- **Real** `trustRegionMinSize`  
  minimum trust region size in the surrogate-based local method (from the `minimum_size` specification in MethodSBL), if the trust region size falls below this threshold the SBL iterations are terminated (note: if kriging is used with SBL, the min trust region size is set to 1.0e-3 in attempt to avoid ill-conditioned matrixes that arise in kriging over small trust regions)

- **Real** `trustRegionContractTrigger`  
  trust region minimum improvement level (ratio of actual to predicted decrease in objective fcn) in the surrogate-based local method (from the `contract_threshold` specification in MethodSBL), the trust region shrinks or is rejected if the ratio is below this value (“eta_1” in the Conn-Gould-Toint trust region book)

- **Real** `trustRegionExpandTrigger`  
  trust region sufficient improvement level (ratio of actual to predicted decrease in objective fcn) in the surrogate-based local method (from the `expand_threshold` specification in MethodSBL), the trust region expands if the ratio is above this value (“eta_2” in the Conn-Gould-Toint trust region book)

- **Real** `trustRegionContract`  
  trust region contraction factor in the surrogate-based local method (from the `contraction_factor` specification in MethodSBL)

- **Real** `trustRegionExpand`
trust region expansion factor in the surrogate-based local method (from the expansion_factor specification in MethodSBL)

- short surrBasedLocalSubProbObj
  SBL approximate subproblem objective: ORIGINAL_PRIMARY, SINGLE_OBJECTIVE, LAGRANGIAN_OBJECTIVE, or AUGMENTED_LAGRANGIAN_OBJECTIVE.

- short surrBasedLocalSubProbCon
  SBL approximate subproblem constraints: NO_CONSTRAINTS, LINEARIZED_CONSTRAINTS, or ORIGINAL_CONSTRAINTS.

- short surrBasedLocalMeritFn
  SBL merit function type: BASIC_PENALTY, ADAPTIVE_PENALTY, BASIC_LAGRANGIAN, or AUGMENTED_LAGRANGIAN.

- short surrBasedLocalAcceptLogic
  SBL iterate acceptance logic: TR_RATIO or FILTER.

- short surrBasedLocalConstrRelax
  SBL constraint relaxation method: NO_RELAX or HOMOTOPY.

- bool surrBasedGlobalReplacePts
  user-specified method for adding points to the set upon which the next surrogate is based in the surrogate-based global method.

- String dlDetails
  string of options for a dynamically linked solver

- void * dlLib
  handle to dynamically loaded library

- int verifyLevel
  the verify_level specification in MethodNPSOLDC

- Real functionPrecision
  the function_precision specification in MethodNPSOLDC and the EPSILON specification in NOMAD

- Real lineSearchTolerance
  the linesearch_tolerance specification in MethodNPSOLDC

- Real absConvTol
  absolute function convergence tolerance

- Real xConvTol
  x-convergence tolerance

- Real singConvTol
  singular convergence tolerance

- Real singRadius
  radius for singular convergence test

- Real falseConvTol
  false-convergence tolerance

- Real initTRRadius
  initial trust radius

- int covarianceType
  kind of covariance required

- bool regressDiag
  whether to print the regression diagnostic vector
• String `searchMethod`
  *the searchMethod specification for Newton and nonlinear interior-point methods in MethodOPTPPDC*

• Real `gradientTolerance`
  *the gradientTolerance specification in MethodOPTPPDC*

• Real `maxStep`
  *the maxStep specification in MethodOPTPPDC*

• Short `meritFn`
  *the meritFunction specification for nonlinear interior-point methods in MethodOPTPPDC*

• Real `stepLenToBoundary`
  *the stepLenToBoundary specification for nonlinear interior-point methods in MethodOPTPPDC*

• Real `centeringParam`
  *the centeringParam specification for nonlinear interior-point methods in MethodOPTPPDC*

• Int `searchSchemeSize`
  *the searchSchemeSize specification for PDS methods in MethodOPTPPDC*

• Real `initStepLength`
  *the initStepLength choice for nonlinearly constrained APPS in MethodAPPSDC*

• Real `contractStepLength`
  *the contractStepLength choice for nonlinearly constrained APPS in MethodAPPSDC*

• Real `threshStepLength`
  *the threshStepLength choice for nonlinearly constrained APPS in MethodAPPSDC*

• String `meritFunction`
  *the meritFunction choice for nonlinearly constrained APPS in MethodAPPSDC*

• Real `constrPenalty`
  *the constrPenalty choice for nonlinearly constrained APPS in MethodAPPSDC*

• Real `smoothFactor`
  *the initial smoothFactor value for nonlinearly constrained APPS in MethodAPPSDC*

• Real `constraintPenalty`
  *the initial constraint_penalty for COLINY methods in MethodAPPS, MethodSCOLIBDIR, MethodSCOLIBPS, MethodSCOLIBSW and MethodSCOLIBEA*

• Bool `constantPenalty`
  *the constantPenalty flag for COLINY methods in MethodSCOLIBPS and MethodSCOLIBSW*

• Real `globalBalanceParam`
  *the globalBalanceParam specification for the DIRECT method in MethodSCOLIBDIR*

• Real `localBalanceParam`
  *the localBalanceParam specification for the DIRECT method in MethodSCOLIBDIR*

• Real `maxBoxSize`
  *the maxBoxsize_limit for the DIRECT method in MethodSCOLIBDIR*

• Real `minBoxSize`
  *the minBoxsize_limit for the DIRECT method in MethodSCOLIBDIR and MethodNCSUDC*

• String `boxDivision`
  *the division setting (major_dimension or all_dimensions) for the DIRECT method in MethodSCOLIBDIR*

• Bool `mutationAdaptive`
The non-adaptive specification for the coliny_ea method in MethodSCOLIBEA

- bool showMiscOptions
  The show_misc_options specification in MethodSCOLIBDC

- StringArray miscOptions
  The misc_options specification in MethodSCOLIBDC

- Real solnTarget
  The solution_target specification in MethodSCOLIBDC

- Real crossoverRate
  The crossover_rate specification for EA methods in MethodSCOLIBEA

- Real mutationRate
  The mutation_rate specification for EA methods in MethodSCOLIBEA

- Real mutationScale
  The mutation_scale specification for EA methods in MethodSCOLIBEA

- Real mutationMinScale
  The min_scale specification for mutation in EA methods in MethodSCOLIBEA

- Real initDelta
  The initial_delta specification for APPS/COBYLA/PS/SW methods in MethodAPPS, MethodSCOLIBCOB, MethodSCOLIBPS, and MethodSCOLIBSW

- Real threshDelta
  The threshold_delta specification for APPS/COBYLA/PS/SW methods in MethodAPPS, MethodSCOLIBCOB, MethodSCOLIBPS, and MethodSCOLIBSW

- Real contractFactor
  The contraction_factor specification for APPS/PS/SW methods in MethodAPPS, MethodSCOLIBPS, and MethodSCOLIBSW

- int newSolnsGenerated
  The new_solutions_generated specification for GA/EPSA methods in MethodSCOLIBEA

- int numberRetained
  The integer assignment to random, chc, or elitist in the replacement_type specification for GA/EPSA methods in MethodSCOLIBEA

- bool expansionFlag
  The no_expansion specification for APPS/PS/SW methods in MethodAPPS, MethodSCOLIBPS, and MethodSCOLIBSW

- int expandAfterSuccess
  The expand_after_success specification for PS/SW methods in MethodSCOLIBPS and MethodSCOLIBSW

- int contractAfterFail
  The contract_after_failure specification for the SW method in MethodSCOLIBSW

- int mutationRange
  The mutation_range specification for the pga_int method in MethodSCOLIBEA

- int totalPatternSize
  The total_pattern_size specification for PS methods in MethodSCOLIBPS

- bool randomizeOrderFlag
  The stochastic specification for the PS method in MethodSCOLIBPS

- String selectionPressure
  The fitness_type specification for EA methods in MethodSCOLIBEA
• String replacementType
  the replacement_type specification for EA methods in MethodSCOLIBEA

• String crossoverType
  the crossover_type specification for EA methods in MethodSCOLIBEA

• String mutationType
  the mutation_type specification for EA methods in MethodSCOLIBEA

• String exploratoryMoves
  the exploratory_moves specification for the PS method in MethodSCOLIBPS

• String patternBasis
  the pattern_basis specification for APPS/PS methods in MethodAPPS and MethodSCOLIBPS

• String betaSolverName
  beta solvers don't need documentation

• String evalSynchronize
  the synchronization setting for parallel pattern search methods in MethodSCOLIBPS and MethodAPPS

• size_t numCrossPoints
  The number of crossover points or multi-point schemes.

• size_t numParents
  The number of parents to use in a crossover operation.

• size_t numOffspring
  The number of children to produce in a crossover operation.

• String fitnessType
  the fitness assessment operator to use.

• String convergenceType
  The means by which this JEGA should converge.

• Real percentChange
  The minimum percent change before convergence for a fitness tracker converger.

• size_t numGenerations
  The number of generations over which a fitness tracker converger should track.

• Real fitnessLimit
  The cutoff value for survival in fitness limiting selectors (e.g., below_limit selector).

• Real shrinkagePercent
  The minimum percentage of the requested number of selections that must take place on each call to the selector (0, 1).

• String nichingType
  The niching type.

• RealVector nicheVector
  The discretization percentage along each objective.

• size_t numDesigns
  The maximum number of designs to keep when using the max_designs nicher.

• String postProcessorType
  The post processor type.

• RealVector distanceVector
  The discretization percentage along each objective.
• **String** `initializationType`  
  *The means by which the JEGA should initialize the population.*  
• **String** `flatFile`  
  *The filename to use for initialization.*  
• **String** `logFile`  
  *The filename to use for logging.*  
• **int** `populationSize`  
  *The population size specification for GA methods in MethodSCOLIBEA*  
• **bool** `printPopFlag`  
  *The print_pop_flag to set the printing of the population at each generation.*  
• **Real** `volBoxSize`  
  *The volume_boxsize_limit for the DIRECT method in MethodNCSUDC*  
• **int** `numSymbols`  
  *The symbols specification for DACE methods*  
• **bool** `mainEffectsFlag`  
  *The main_effects specification for sampling methods in MethodDDACE)*  
• **bool** `latinizeFlag`  
  *The latinize specification for FSU QMC and CVT methods in MethodFSUDACE*  
• **bool** `volQualityFlag`  
  *The quality_metrics specification for sampling methods (FSU QMC and CVT methods in MethodFSUDACE)*  
• **IntVector** `sequenceStart`  
  *The sequenceStart specification in MethodFSUDACE*  
• **IntVector** `sequenceLeap`  
  *The sequenceLeap specification in MethodFSUDACE*  
• **IntVector** `primeBase`  
  *The primeBase specification in MethodFSUDACE*  
• **int** `numTrials`  
  *The numTrials specification in MethodFSUDACE*  
• **String** `trialType`  
  *The trial_type specification in MethodFSUDACE*  
• **int** `randomSeed`  
  *The seed specification for COLINY, NonD, & DACE methods*  
• **Real** `initMeshSize`  
  *The initMeshSize choice for NOMAD in MethodNOMADDC*  
• **Real** `minMeshSize`  
  *The minMeshSize choice for NOMAD in MethodNOMADDC*  
• **String** `historyFile`  
  *The HISTORY_FILE specification for NOMAD*  
• **String** `displayFormat`  
  *The DISPLAY_STATS specification for NOMAD*  
• **Real** `vns`  
  *The VNS specification for NOMAD*  
• **int** `neighborOrder`
the `NEIGHBOR_ORDER` specification for NOMAD

- `bool showAllEval`
  the `DISPLAY_ALL_EVAL` specification for NOMAD

- `String useSurrogate`
  the `HAS_SGTE` specification for NOMAD

- `int numSamples`
  the `samples` specification for NonD & DACE methods

- `bool fixedSeedFlag`
  flag for fixing the value of the seed among different NonD/DACE sample sets. This results in the use of the same sampling stencil/pattern throughout an execution with repeated sampling.

- `bool fixedSequenceFlag`
  flag for fixing the sequence for Halton or Hammersley QMC sample sets. This results in the use of the same sampling stencil/pattern throughout an execution with repeated sampling.

- `bool vbdFlag`
  the `var_based_decomp` specification for a variety of sampling methods

- `Real vbdDropTolerance`
  the `var_based_decomp` tolerance for omitting index output

- `bool backfillFlag`
  the `backfill` option allows one to augment in LHS sample by enforcing the addition of unique discrete variables to the sample

- `bool pcaFlag`
  Flag to specify the calculation of principal components when using LHS.

- `Real percentVarianceExplained`
  The percentage of variance explained by using a truncated number of principal components in PCA.

- `bool wilksFlag`
  Flag to specify use of Wilks formula to calculate num samples.

- `unsigned short wilksOrder`
  Wilks order parameter.

- `Real wilksConfidenceLevel`
  Wilks confidence interval parameter.

- `short wilksSidedInterval`
  Wilks sided interval type.

- `unsigned short vbdOrder`
  a sub-specification of vbdFlag: interaction order limit for calculation/output of component VBD indices

- `short covarianceControl`
  restrict the calculation of a full response covariance matrix for high dimensional outputs: \{DEFAULT,DIAGONAL,FULL\}_COVARIANCE

- `String rngName`
  the basic random-number generator for NonD

- `short refinementType`
  refinement type for stochastic expansions from dimension refinement keyword group

- `short refinementControl`
  refinement control for stochastic expansions from dimension refinement keyword group

- `short nestingOverride`
override for default point nesting policy: \texttt{NO\_NESTING\_OVER\_RID}, \texttt{NESTED}, or \texttt{NON\_NESTED}

- short \texttt{growthOverride}
  override for default point growth restriction policy: \texttt{NO\_GROWTH\_OVER\_RIDE}, \texttt{RESTRICTED}, or \texttt{UNRESTRICTED}

- short \texttt{expansionType}
  enumeration for \texttt{u-space} type that defines \texttt{u-space} variable targets for probability space transformations: \texttt{EXTENDED\_U} (default), \texttt{ASKEY\_U}, \texttt{STD\_NORMAL\_U}, or \texttt{STD\_UNIFORM\_U}

- bool \texttt{piecewiseBasis}
  boolean indicating presence of \texttt{piecewise} keyword

- short \texttt{expansionBasisType}
  enumeration for type of basis in sparse grid interpolation (\texttt{Pecos::\{NODAL,HIERARCHICAL\}_INTERPOLANT}) or regression (\texttt{Pecos::\{TENSOR\_PRODUCT,TOTAL\_ORDER,ADAPTED\}_BASIS}).

- UShortArray \texttt{expansionOrder}
  the \texttt{expansion\_order} specification in Method\_Non\_DPCE

- SizetArray \texttt{expansionSamples}
  the \texttt{expansion\_samples} specification in Method\_Non\_DPCE

- String \texttt{expansionSampleType}
  allows for incremental PCE construction using the \texttt{incremental\_lhs} specification in Method\_Non\_DPCE

- UShortArray \texttt{quadratureOrder}
  the \texttt{quadrature\_order} specification in Method\_Non\_DPCE and Method\_Non\_DSC

- UShortArray \texttt{sparseGridLevel}
  the \texttt{sparse\_grid\_level} specification in Method\_Non\_DPCE, Method\_Non\_DSC, and other stochastic expansion-enabled methods

- RealVector \texttt{anisoDimPref}
  the \texttt{dimension\_preference} specification for tensor and sparse grids and expansion orders in Method\_Non\_DPCE and Method\_Non\_DSC

- unsigned short \texttt{cubIntOrder}
  the \texttt{cubature\_integrand} specification in Method\_Non\_DPCE

- SizetArray \texttt{collocationPoints}
  the \texttt{collocation\_points} specification in Method\_Non\_DPCE

- Real \texttt{collocationRatio}
  the \texttt{collocation\_ratio} specification in Method\_Non\_DPCE

- Real \texttt{collocRatioTermsOrder}
  order applied to the number of expansion terms when applying or computing the collocation ratio within regression PCE; based on the \texttt{ratio\_order} specification in Method\_Non\_DPCE

- short \texttt{regressionType}
  type of regression: LS, OMP, BP, BPDN, LARS, or LASSO

- short \texttt{lsRegressionType}
  type of least squares regression: SVD or \texttt{EQ\_CON\_QR}

- RealVector \texttt{regressionNoiseTol}
  noise tolerance(s) for OMP, BPDN, LARS, and LASSO

- Real \texttt{regressionL2Penalty}
  L2 regression penalty for a variant of LASSO known as the elastic net method (default of 0 gives standard LASSO)

- bool \texttt{crossValidation}
flag indicating the use of cross-validation across expansion orders (given a prescribed maximum order) and, for some methods, noise tolerances

- `bool crossValidNoiseOnly`
  flag indicating the restriction of cross-validation to estimate only the most effective noise tolerance; used to reduce cost from performing CV over both noise tolerances and expansion orders

- `unsigned short adaptedBasisAdvancements`
  initial grid level for the ADAPTED_BASIS_EXPANDING_FRONT approach to defining the candidate basis for sparse recovery (compressed sensing)

- `bool normalizedCoeffs`
  flag indicating the output of PCE coefficients corresponding to normalized basis polynomials

- `String pointReuse`
  allows PCE construction to reuse points from previous sample sets or data import using the `reuse_points` specification in MethodNonDPCE

- `bool tensorGridFlag`
  flag for usage of a sub-sampled set of tensor-product grid points within regression PCE; based on the `tensor_grid` specification in MethodNonDPCE

- `UShortArray tensorGridOrder`
  order of tensor-product grid points that are sub-sampled within orthogonal least interpolation PCE; based on the `tensor_grid` specification in MethodNonDPCE

- `String importExpansionFile`
  the `import_expansion_file` specification in MethodNonDPCE

- `String exportExpansionFile`
  the `export_expansion_file` specification in MethodNonDPCE

- `unsigned short sampleType`
  the `sample_type` specification in MethodNonDMC, MethodNonDPCE, and MethodNonDSC

- `bool dOptimal`
  whether to generate D-optimal designs

- `size_t numCandidateDesigns`
  number of candidate designs in D-optimal design selection

- `unsigned short reliabilitySearchType`
  the type of limit state search in MethodNonDLocalRel (x_taylor_mean, x_taylor_mpp, x_two_point, u_taylor_mean, u_taylor_mpp, u_two_point, or no_approx) or MethodNonDGlobalRel (x_gaussian_process or u_gaussian_process)

- `String reliabilityIntegration`
  the first_order or second_order integration selection in MethodNonDLocalRel

- `unsigned short integrationRefine`
  the import, adapt_import, or mm_adapt_import integration refinement selection in MethodNonDLocalRel, MethodNonDPCE, and MethodNonDSC

- `IntVector refineSamples`
  Sequence of refinement samples, e.g., the size of the batch (e.g. number of supplemental points added) to be added to be added to the build points for an emulator at each iteration.

- `SizetArray pilotSamples`
  the `pilot_samples` selection in MethodMultilevelMC

- `short finalMomentsType`
  the final_moments specification in MethodNonD
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- short `distributionType`
  the distribution cumulative or complementary specification in MethodNonD

- short `responseLevelTarget`
  the compute probabilities, reliabilities, or gen.reliabilities specification in MethodNonD

- short `responseLevelTargetReduce`
  the system series or parallel specification in MethodNonD

- RealVectorArray `responseLevels`
  the response_levels specification in MethodNonD

- RealVectorArray `probabilityLevels`
  the probability_levels specification in MethodNonD

- RealVectorArray `reliabilityLevels`
  the reliability_levels specification in MethodNonD

- RealVectorArray `genReliabilityLevels`
  the gen.reliability_levels specification in MethodNonD

- int `chainSamples`
  the number of MCMC chain samples

- int `buildSamples`
  the number of samples to construct an emulator, e.g., for Bayesian calibration methods

- int `samplesOnEmulator`
  number of samples to perform on emulator

- int `emulatorOrder`
  The total order to be used in construction of a VPS surrogate.

- short `emulatorType`
  the emulator specification in MethodNonDBayesCalib

- String `mcmcType`
  the mcmc type specification in MethodNonDBayesCalib

- bool `standardizedSpace`
  use of standardized probability spaces for MCMC within Bayesian inference

- bool `adaptPosteriorRefine`
  flag indicating adaptive refinement of the emulator in regions of high posterior probability

- bool `logitTransform`
  flag indicating user activation of logit transform option within QUESO

- bool `gpmsaNormalize`
  whether to apply GPMSA-internal normalization

- bool `posteriorStatsKL`
  flag indicating the calculation of KL divergence between prior and posterior in Bayesian methods

- bool `posteriorStatsMutual`
  flag indicating the calculation of mutual information between prior and posterior in Bayesian methods

- unsigned short `preSolveMethod`
  the method used for performing a pre-solve for the MAP point

- String `proposalCovType`
  the type of proposal covariance: user, derivatives, or prior

- int `proposalCovUpdates`
number of updates of the proposal covariance from computing the misfit Hessian using residual values and derivatives

- **String** `proposalCovInputType`
  the format of proposal covariance input: diagonal or matrix

- **RealVector** `proposalCovData`
  raw list of real data for the proposal covariance

- **String** `proposalCovFile`
  file from which to read proposal covariance in diagonal or matrix format

- **String** `quesoOptionsFilename`
  file containing advanced QUESO option overrides

- **String** `fitnessMetricType`
  the fitness metric type specification in MethodNonDAdaptive

- **String** `batchSelectionType`
  the batch selection type specification in MethodNonDAdaptive

- **String** `lipschitzType`
  the Lipschitz type specification in MethodNonDPOFDarts (e.g. either local or global estimation)

- **unsigned short** `calibrateErrorMode`
  calibration mode for observation error multipliers (CALIBRATE_*)

- **RealVector** `hyperPriorAlphas`
  hyperparameters inverse gamma prior alphas

- **RealVector** `hyperPriorBetas`
  hyperparameters inverse gamma prior alphas

- **int** `burnInSamples`
  number of MCMC samples to discard from acceptance chain

- **int** `subSamplingPeriod`
  period or skip in post-processing the acceptance chain

- **bool** `calModelDiscrepancy`
  flag to calculate model discrepancy

- **size_t** `numPredConfigs`
  number of prediction configurations at which to calculate model discrepancy

- **RealVector** `predictionConfigList`
  list of prediction configurations at which to calculate model discrepancy

- **String** `importPredConfigs`
  whether to import prediction configurations at which to calculate model discrepancy

- **unsigned short** `importPredConfigFormat`
  tabular format for prediction configurations import file

- **String** `discrepancyType`
  specify type of model discrepancy formulation

- **short** `approxCorrectionOrder`
  correction order for either gaussian process or polynomial model discrepancy calculations: 0 (=constant), 1 (=linear), 2 (=quadratic)

- **String** `exportCorrModelFile`
  specify the name of file to which corrected model (model+discrepancy) calculations are output
• unsigned short exportCorrModelFormat
  tabular format for corrected model (model+discrepancy) export file
• String exportCorrVarFile
  specify the name of file to which corrected model variance calculations are output
• unsigned short exportCorrVarFormat
  tabular format for corrected model variance export file
• String exportDiscrepFile
  specify the name of file to which discrepancy calculations are output
• unsigned short exportDiscrepFormat
  tabular format for model discrepancy export file
• bool adaptExpDesign
  whether to perform adaptive Bayesian design of experiments
• String importCandPtsFile
  whether to import candidate design points for adaptive Bayesian experimental design
• unsigned short importCandFormat
  tabular format for the candidate design points import file
• size_t numCandidates
  number of candidate designs for adaptive Bayesian experimental design
• int maxHifiEvals
  maximum number of highfidelity model runs to be used for adaptive Bayesian experimental design
• int numChains
  number of concurrent chains
• int numCR
  number of CR-factors
• int crossoverChainPairs
  number of crossover chain pairs
• Real grThreshold
  threshold for the Gelman-Rubin statistic
• int jumpStep
  how often to perform a long jump in generations
• String dataDistType
  the type of data distribution: kde, or gaussian
• String dataDistCovInputType
  the format of data distribution gaussian covariance input: diagonal or matrix
• RealVector dataDistMeans
  raw list of real data for the data distribution gaussian means
• RealVector dataDistCovariance
  raw list of real data for the data distribution gaussian covariance
• String dataDistFile
  file from which to read data distribution data (covariance or samples)
• String posteriorDensityExportFilename
  The filename of the export file containing an arbitrary set of samples and their corresponding density values.
• String posteriorSamplesExportFilename
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- **String** `posteriorSamplesImportFilename`
  The filename of the import file containing samples at which the posterior will be evaluated.

- **bool** `generatePosteriorSamples`
  Flag specifying whether to generate random samples from the posterior.

- **bool** `evaluatePosteriorDensity`
  Flag specifying whether to evaluate the posterior density at a set of samples.

- **RealVector** `finalPoint`
  the final_point specification in MethodPSVPS

- **RealVector** `stepVector`
  the step_vector specification in MethodPSVPS and MethodPSCPS

- **int** `numSteps`
  the num_steps specification in MethodPSVPS

- **IntVector** `stepsPerVariable`
  the deltas_per_variable specification in MethodPSCPS

- **RealVector** `listOfPoints`
  the list_of_points specification in MethodPSLPS

- **String** `pstudyFilename`
  the import_points_file spec for a file-based parameter study

- **unsigned short** `pstudyFileFormat`
  tabular format for the parameter study points file

- **bool** `pstudyFileActive`
  whether to import active variables only

- **UShortArray** `varPartitions`
  the partitions specification for PStudy method in MethodPSMPS

- **Real** `refinementRate`
  rate of mesh refinement in Richardson extrapolation

- **String** `importBuildPtsFile`
  the file name from the import_build_points_file specification

- **unsigned short** `importBuildFormat`
  tabular format for the build point import file

- **bool** `importBuildActive`
  whether to import active variables only

- **String** `importApproxPtsFile`
  the file name from the import_approx_points_file specification

- **unsigned short** `importApproxFormat`
  tabular format for the approx point import file

- **bool** `importApproxActive`
  whether to import active variables only

- **String** `exportApproxPtsFile`
  the file name from the export_approx_points_file specification

- **unsigned short** `exportApproxFormat`
  tabular format for the approx point export file
13.33. DATAMODEL CLASS REFERENCE

- **String exportMCMCPtsFile**
  the file name from the `export_mcmc_points_file` specification

- **bool exportSampleSeqFlag**
  flag for exporting the sequence of sample increments within multilevel sampling from the `export_sample_sequence` specification

- **unsigned short exportSamplesFormat**
  tabular format for the MCMC chain and MLMC sample sequence exports

**Private Member Functions**

- **DataMethodRep ()**
  constructor

- **~DataMethodRep ()**
  destructor

- **void write (std::ostream &s) const**
  write a DataInterfaceRep object to an std::ostream

- **void read (MPIUnpackBuffer &s)**
  read a DataInterfaceRep object from a packed MPI buffer

- **void write (MPIPackBuffer &s) const**
  write a DataInterfaceRep object to a packed MPI buffer

**Private Attributes**

- **int referenceCount**
  number of handle objects sharing this dataMethodRep

**Friends**

- **class DataMethod**
  the handle class can access attributes of the body class directly

13.32.1 Detailed Description

Body class for method specification data.

The DataMethodRep class is used to contain the data from a method keyword specification. Default values are managed in the DataMethodRep constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::dataMethodList is private.

The documentation for this class was generated from the following files:

- DataMethod.hpp
- DataMethod.cpp

13.33 DataModel Class Reference

Handle class for model specification data.
Public Member Functions

- **DataModel ()**
  
  *constructor*

- **DataModel (const DataModel &)**
  
  *copy constructor*

- **~DataModel ()**
  
  *destructor*

- **DataModel & operator= (const DataModel &)**
  
  *assignment operator*

- **void write (std::ostream &s) const**
  
  *write a DataModel object to an std::ostream*

- **void read (MPIUnpackBuffer &s)**
  
  *read a DataModel object from a packed MPI buffer*

- **void write (MPIPackBuffer &s) const**
  
  *write a DataModel object to a packed MPI buffer*

- **DataModelRep * data_rep ()**
  
  *return dataModelRep*

Static Public Member Functions

- **static bool id_compare (const DataModel &dm, const std::string &id)**
  
  *compares the idModel attribute of DataModel objects*

Private Attributes

- **DataModelRep * dataModelRep**
  
  *pointer to the body (handle-body idiom)*

Friends

- **class ProblemDescDB**
- **class NIDRProblemDescDB**

13.33.1 Detailed Description

Handle class for model specification data.

The DataModel class is used to provide a memory management handle for the data in DataModelRep. It is populated by IDRProblemDescDB::model_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataModel objects is maintained in ProblemDescDB::dataModelList, one for each model specification in an input file.

The documentation for this class was generated from the following files:

- DataModel.hpp
- DataModel.cpp
13.34 DataModelRep Class Reference

Body class for model specification data.

Public Attributes

- **String idModel**
  
  string identifier for the model specification data set (from the id_model specification in ModelIndControl)

- **String modelType**
  
  model type selection: single, surrogate, or nested (from the model type specification in ModelIndControl)

- **String variablesPointer**
  
  string pointer to the variables specification to be used by this model (from the variables_pointer specification in ModelIndControl)

- **String interfacePointer**
  
  string pointer to the interface specification to be used by this model (from the interface_pointer specification in ModelSingle and the optional_interface_pointer specification in ModelNested)

- **String responsesPointer**
  
  string pointer to the responses specification to be used by this model (from the responses_pointer specification in ModelIndControl)

- **bool hierarchicalTags**
  
  whether this model and its children will add hierarchy-based tags to eval ids

- **String subMethodPointer**
  
  pointer to a sub-iterator used for global approximations (from the dace_method_pointer specification in ModelSurrG) or by nested models (from the sub_method_pointer specification in ModelNested)

- **String solutionLevelControl**
  
  (state) variable identifier that defines a set or range of solution level controls (space/time discretization levels, iterative convergence tolerances, etc.) for defining a secondary hierarchy of fidelity within the scope of a single model form (from solution_level_control specification; see also ordered_model_fidelities)

- **RealVector solutionLevelCost**
  
  array of relative simulation costs corresponding to each of the solution levels (from solution_level_cost specification; see also solution_level_control); a scalar input is interpreted as a constant cost multiplier to be applied recursively

- **IntSet surrogateFnIndices**
  
  array specifying the response function set that is approximated

- **String surrogateType**
  
  the selected surrogate type: local_taylor, multipoint_tana, global_neural_network, mars, orthogonal_polynomial, gaussian, polynomial, kriging, or hierarchical

- **String actualModelPointer**
  
  pointer to the model specification for constructing the truth model used in constructing surrogates (from the actual_model_pointer specification in ModelSurrL and ModelSurrMP)

- **StringArray orderedModelPointers**
  
  an ordered list of model pointers (low to high) corresponding to a hierarchy of modeling fidelity (from the ordered_model_fidelities specification in ModelSurrH)

- **int pointsTotal**
  
  user-specified lower bound on total points with which to build the model (if reuse_points < pointsTotal, new samples will make up the difference)
• short pointsManagement
  points management configuration for DataFitSurrModel: DEFAULT_POINTS, MINIMUM_POINTS, or RECOMMENDED_POINTS
• String approxPointReuse
  sample reuse selection for building global approximations: none, all, region, or file (from the reuse_samples specification in ModelSurrG)
• String importBuildPtsFile
  the file name from the import_build_points_file specification in ModelSurrG
• unsigned short importBuildFormat
  tabular format for the build point import file
• bool importBuildActive
  whether to import active variables only
• String exportApproxPtsFile
  the file name from the export_approx_points_file specification in ModelSurrG
• unsigned short exportApproxFormat
  tabular format for the approx point export file
• bool exportSurrogate
  Option to turn on surrogate model export (export_model)
• String modelExportPrefix
  the filename prefix for export_model
• unsigned short modelExportFormat
  Format selection for export_model.
• short approxCorrectionType
  correction type for global and hierarchical approximations: NO_CORRECTION, ADDITIVE_CORRECTION, MULTIPLICATIVE_CORRECTION, or COMBINED_CORRECTION (from the correction specification in ModelSurrG and ModelSurrH)
• short approxCorrectionOrder
  correction order for global and hierarchical approximations: 0, 1, or 2 (from the correction specification in ModelSurrG and ModelSurrH)
• bool modelUseDerivsFlag
  flags the use of derivatives in building global approximations (from the use_derivatives specification in ModelSurrG)
• short polynomialOrder
  scalar integer indicating the order of the polynomial approximation (1=linear, 2=quadratic, 3=cubic; from the polynomial specification in ModelSurrG)
• RealVector krigingCorrelations
  vector of correlations used in building a kriging approximation (from the correlations specification in ModelSurrG)
• String krigingOptMethod
  optimization method to use in finding optimal correlation parameters: none, sampling, local, global
• short krigingMaxTrials
  maximum number of trials in optimization of kriging correlations
• RealVector krigingMaxCorrelations
  upper bound on kriging correlation vector
• RealVector krigingMinCorrelations
lower bound on kriging correlation vector

- Real `krigingNugget`
  nugget value for kriging
- short `krigingFindNugget`
  option to have Kriging find the best nugget value to use
- short `mlsWeightFunction`
  weight function for moving least squares approximation
- short `rbfBases`
  bases for radial basis function approximation
- short `rbfMaxPts`
  maximum number of points for radial basis function approximation
- short `rbfMaxSubsets`
  maximum number of subsets for radial basis function approximation
- short `rbfMinPartition`
  minimum partition for radial basis function approximation
- short `marsMaxBases`
  maximum number of bases for MARS approximation
- String `marsInterpolation`
  interpolation type for MARS approximation
- short `annRandomWeight`
  random weight for artificial neural network approximation
- short `annNodes`
  number of nodes for artificial neural network approximation
- Real `annRange`
  range for artificial neural network approximation
- bool `domainDecomp`
  whether domain decomposition is enabled
- String `decompCellType`
  type of local cell of domain decomp
- int `decompSupportLayers`
  number of support layers for each local basis function
- bool `decompDiscontDetect`
  whether discontinuity detection is enabled
- Real `discontJumpThresh`
  function value (jump) threshold for discontinuity detection in domain decomp
- Real `discontGradThresh`
  gradient threshold for discontinuity detection in domain decomp
- String `trendOrder`
  scalar integer indicating the order of the Gaussian process mean (0=constant, 1=linear, 2=quadratic, 3=cubic);
  from the gaussian_process specification in ModelSurrG)
- bool `pointSelection`
  flag indicating the use of point selection in the Gaussian process
- StringArray `diagMetrics`
List of diagnostic metrics the user requests to assess the goodness of fit for a surrogate model.

- **bool crossValidateFlag**
  - flag indicating the use of cross validation on the metrics specified
- **int numFolds**
  - number of folds to perform in cross validation
- **Real percentFold**
  - percentage of data to withhold for cross validation process
- **bool pressFlag**
  - flag indicating the use of PRESS on the metrics specified
- **String importChallengePtsFile**
  - the file name from the `challenge_points_file` specification in `ModelSurrG`
- **unsigned short importChallengeFormat**
  - tabular format of the challenge data file
- **bool importChallengeActive**
  - whether to import active variables only
- **String optionalInterfRespPointer**
  - string pointer to the responses specification used by the optional interface in nested models (from the `optional_interface_responses_pointer` specification in `ModelNested`)
- **StringArray primaryVarMaps**
  - the primary variable mappings used in nested models for identifying the lower level variable targets for inserting top level variable values (from the `primary_variable_mapping` specification in `ModelNested`)
- **StringArray secondaryVarMaps**
  - the secondary variable mappings used in nested models for identifying the (distribution) parameter targets within the lower level variables for inserting top level variable values (from the `secondary_variable_mapping` specification in `ModelNested`)
- **RealVector primaryRespCoeffs**
  - the primary response mapping matrix used in nested models for weighting contributions from the sub-iterator responses in the top level (objective) functions (from the `primary_response_mapping` specification in `ModelNested`)
- **RealVector secondaryRespCoeffs**
  - the secondary response mapping matrix used in nested models for weighting contributions from the sub-iterator responses in the top level (constraint) functions (from the `secondary_response_mapping` specification in `ModelNested`)
- **int subMethodServers**
  - number of servers for concurrent sub-iterator parallelism
- **int subMethodProcs**
  - number of processors for each concurrent sub-iterator partition
- **short subMethodScheduling**
  - scheduling approach for concurrent sub-iterator parallelism: `{DEFAULT,MASTER,PEER}_SCHEDULING`
- **int initialSamples**
  - initial samples to build the subspace model
- **unsigned short subspaceSampleType**
  - sampling method for building the subspace model
- **IntVector refineSamples**
  - refinement samples to add in each batch
• int maxIterations
  maximum number of subspace build iterations
• Real convergenceTolerance
  convergence tolerance on build process
• bool subspaceIdBingLi
  Flag to use Bing Li method to identify active subspace dimension.
• bool subspaceIdConstantine
  Flag to use Constantine method to identify active subspace dimension.
• bool subspaceIdEnergy
  Flag to use eigenvalue energy method to identify active subspace dimension.
• bool subspaceBuildSurrogate
  Flag to build surrogate over active subspace.
• int subspaceDimension
  Size of subspace.
• unsigned short subspaceNormalization
  Normalization to use when forming a subspace with multiple response functions.
• int numReplicates
  Number of bootstrap samples for subspace identification.
• bool subspaceIdCV
  Flag to use cross validation to identify active subspace dimension.
• Real relTolerance
  relative tolerance used by cross validation subspace dimension id method
• Real decreaseTolerance
  decrease tolerance used by cross validation subspace dimension id method
• int subspaceCVMaxRank
  maximum rank considered by cross validation subspace dimension id method
• bool subspaceCVIncremental
  flag to use incremental dimension estimation in the cross validation metric
• unsigned short subspaceIdCVMethod
  Contains which cutoff method to use in the cross validation metric.
• bool autoRefine
  whether automatic surrogate refinement is enabled
• int maxFunctionEvals
  maximum evals in refinement
• String refineCVMetric
  metric to use in cross-validation guided refinement
• int softConvergenceLimit
  max number of iterations in refinement without improvement
• int refineCVFolds
  number of cross-validation folds in guided refinement
• unsigned short adaptedBasisSparseGridLev
  sparse grid level for low-order PCE used to compute rotation matrix within adapted basis approach to dimension reduction
• unsigned short \texttt{adaptedBasisExpOrder}
  
  expansion order for low-order PCE used to compute rotation matrix within adapted basis approach to dimension reduction

• Real \texttt{adaptedBasisCollocRatio}
  
  collocation ratio for low-order PCE used to compute rotation matrix within adapted basis approach to dimension reduction

• unsigned short \texttt{randomFieldIdForm}
  
  Contains which type of random field model.

• unsigned short \texttt{analyticCovIdForm}
  
  Contains which type of analytic covariance function.

• Real \texttt{truncationTolerance}
  
  truncation tolerance on build process: percent variance explained

• String \texttt{propagationModelPointer}
  
  pointer to the model through which to propagate the random field

• String \texttt{rfDataFileName}
  
  File from which to build the random field.

**Private Member Functions**

• \texttt{DataModelRep ()}
  
  constructor

• \texttt{\sim DataModelRep ()}
  
  destructor

• void \texttt{write (std::ostream \&s) const}
  
  write a \texttt{DataModelRep} object to an std::ostream

• void \texttt{read (MPIUnpackBuffer \&s)}
  
  read a \texttt{DataModelRep} object from a packed MPI buffer

• void \texttt{write (MPIPackBuffer \&s) const}
  
  write a \texttt{DataModelRep} object to a packed MPI buffer

**Private Attributes**

• int \texttt{referenceCount}
  
  number of handle objects sharing this dataModelRep

**Friends**

• class \texttt{DataModel}
  
  the handle class can access attributes of the body class directly
13.34.1 Detailed Description

Body class for model specification data.

The `DataModelRep` class is used to contain the data from a model keyword specification. Default values are managed in the `DataModelRep` constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within `ProblemDescDB` since `ProblemDescDB::dataModelList` is private.

The documentation for this class was generated from the following files:

- DataModel.hpp
- DataModel.cpp

13.35 DataResponses Class Reference

Handle class for responses specification data.

Public Member Functions

- `DataResponses ()`
  constructor
- `DataResponses (const DataResponses &)`
  copy constructor
- `~DataResponses ()`
  destructor
- `DataResponses & operator= (const DataResponses &)`
  assignment operator
- `void write (std::ostream &s) const`
  write a `DataResponses` object to an `std::ostream`
- `void read (MPIUnpackBuffer &s)`
  read a `DataResponses` object from a packed MPI buffer
- `void write (MPIPackBuffer &s) const`
  write a `DataResponses` object to a packed MPI buffer
- `DataResponsesRep * data_rep ()`
  return `dataRespRep`

Static Public Member Functions

- `static bool id_compare (const DataResponses &dr, const std::string &id)`
  compares the idResponses attribute of `DataResponses` objects

Private Attributes

- `DataResponsesRep * dataRespRep`
  pointer to the body (handle-body idiom)

Friends

- class `ProblemDescDB`
- class `NIDRProblemDescDB`
13.35.1 Detailed Description

Handle class for responses specification data.

The DataResponses class is used to provide a memory management handle for the data in DataResponsesRep. It is populated by IDRProblemDescDB::responses_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataResponses objects is maintained in ProblemDescDB::dataResponsesList, one for each responses specification in an input file.

The documentation for this class was generated from the following files:

- DataResponses.hpp
- DataResponses.cpp

13.36 DataResponsesRep Class Reference

Body class for responses specification data.

Public Attributes

- String idResponses
  
  string identifier for the responses specification data set (from the id_responses specification in RespSetId)

- StringArray responseLabels
  
  the response labels array (from the response_descriptors specification in RespLabels)

- size_t numObjectiveFunctions
  
  number of objective functions (from the num_objective_functions specification in RespFnOpt)

- size_t numLeastSqTerms
  
  number of least squares terms (from the num_calibration_terms specification in RespFnLS)

- size_t numNonlinearIneqConstraints
  
  number of nonlinear inequality constraints (from the num_nonlinear_inequality_constraints specification in RespFnOpt)

- size_t numNonlinearEqConstraints
  
  number of nonlinear equality constraints (from the num_nonlinear_equality_constraints specification in RespFnOpt)

- size_t numResponseFunctions
  
  number of generic response functions (from the num_response_functions specification in RespFnGen)

- size_t numScalarObjectiveFunctions
  
  scalar_objectives: number of objective functions which are scalar

- size_t numScalarLeastSqTerms
  
  scalar_calibration_terms: number of calibration terms which are scalar

- size_t numScalarNonlinearIneqConstraints
  
  number of scalar nonlinear inequality constraints (from the num_scalar_nonlinear_inequality_constraints specification in RespFnOpt)

- size_t numScalarNonlinearEqConstraints
  
  number of scalar nonlinear equality constraints (from the num_scalar_nonlinear_equality_constraints specification in RespFnOpt)

- size_t numScalarResponseFunctions
  
  scalar_responses: number of response functions which are scalar
• `size_t numFieldObjectiveFunctions`
  
  field_objectives: number of objective functions which are field-valued

• `size_t numFieldLeastSqTerms`
  
  field_calibration_terms: number of calibration terms which are field-valued

• `size_t numFieldNonlinearIneqConstraints`
  
  number of field nonlinear inequality constraints (from the num_scalar_nonlinear_inequality_constraints specification in RespFnOpt)

• `size_t numFieldNonlinearEqConstraints`
  
  number of field nonlinear equality constraints (from the num_scalar_nonlinear_equality_constraints specification in RespFnOpt)

• `size_t numFieldResponseFunctions`
  
  field_responses: number of response functions which are field-valued

• `StringArray primaryRespFnSense`
  
  optimization sense for each objective function: minimize or maximize

• `RealVector primaryRespFnWeights`
  
  vector of weightings for multiobjective optimization or weighted nonlinear least squares (from the multi_objective_weights specification in RespFnOpt and the least_squares_weights specification in RespFnLS)

• `RealVector nonlinearIneqLowerBnds`
  
  vector of nonlinear inequality constraint lower bounds (from the nonlinear_inequality_lower_bounds specification in RespFnOpt)

• `RealVector nonlinearIneqUpperBnds`
  
  vector of nonlinear inequality constraint upper bounds (from the nonlinear_inequality_upper_bounds specification in RespFnOpt)

• `RealVector nonlinearEqTargets`
  
  vector of nonlinear equality constraint targets (from the nonlinear_equality_targets specification in RespFnOpt)

• `StringArray primaryRespFnScaleTypes`
  
  vector of primary response function scaling types (from the objective_function_scale_types specification in RespFnOpt and the least_squares_term_scale_types specification in RespFnLS)

• `RealVector primaryRespFnScales`
  
  vector of primary response function scaling factors (from the objective_function_scales specification in RespFnOpt and the least_squares_term_scales specification in RespFnLS)

• `StringArray nonlinearIneqScaleTypes`
  
  vector of nonlinear inequality constraint scaling types (from the nonlinear_inequality_scale_types specification in RespFnOpt)

• `RealVector nonlinearIneqScales`
  
  vector of nonlinear inequality constraint scaling factors (from the nonlinear_inequality_scales specification in RespFnOpt)

• `StringArray nonlinearEqScaleTypes`
  
  vector of nonlinear equality constraint scaling types (from the nonlinear_equality_scale_types specification in RespFnOpt)

• `RealVector nonlinearEqScales`
  
  vector of nonlinear equality constraint scaling factors (from the nonlinear_equality_scales specification in RespFnOpt)

• `bool calibrationDataFlag`
whether calibration data was specified

- `size_t numExperiments`
  number of distinct experiments in experimental data

- `size_t numExpConfigVars`
  number of experimental configuration vars (state variables) in each row of data

- `RealVector expConfigVars`
  list of num_experiments x num_config_vars configuration variable values

- `bool interpolateFlag`
  whether one should interpolate between the experiment and simulation field data

- `RealVector expObservations`
  list of num_calibration_terms observation data

- `RealVector expStdDeviations`
  list of 1 or num_calibration_terms observation standard deviations

- `String scalarDataFileName`
  name of experimental data file containing response data (with optional state variable and sigma data) to read

- `unsigned short scalarDataFormat`
  tabular format of the scalar data file

- `String gradientType`
  gradient type: none, numerical, analytic, or mixed (from the no_gradients, numerical_gradients, analytic_gradients, and mixed_gradients specifications in RespGrad)

- `String hessianType`
  Hessian type: none, numerical, quasi, analytic, or mixed (from the no_hessians, numerical_hessians, quasi_hessians, analytic_hessians, and mixed_hessians specifications in RespHess)

- `bool ignoreBounds`
  option to ignore bounds when doing finite differences (default is to honor bounds)

- `bool centralHess`
  Temporary(?) option to use old 2nd-order diffs when computing finite-difference Hessians; default is forward differences.

- `String quasiHessianType`
  quasi-Hessian type: bfgs, damped_bfgs, or sr1 (from the bfgs and sr1 specifications in RespHess)

- `String methodSource`
  numerical gradient method source: dakota or vendor (from the method_source specification in RespGradNum and RespGradMixed)

- `String intervalType`
  numerical gradient interval type: forward or central (from the interval_type specification in RespGradNum and RespGradMixed)

- `RealVector fdGradStepSize`
  vector of finite difference step sizes for numerical gradients, one step size per active continuous variable, used in computing 1st-order forward or central differences (from the fd_gradient_step_size specification in RespGradNum and RespGradMixed)

- `String fdGradStepType`
  type of finite difference step to use for numerical gradient: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x

- `RealVector fdHessStepSize`
vector of finite difference step sizes for numerical Hessians, one step size per active continuous variable, used in computing 1st-order gradient-based differences and 2nd-order function-based differences (from the fd_hessian_step_size specification in RespHessNum and RespHessMixed)

- String fdHessStepType
type of finite difference step to use for numerical Hessian: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x

- IntSet idNumericalGrads
  mixed gradient numerical identifiers (from the id_numerical_gradients specification in RespGradMixed)

- IntSet idAnalyticGrads
  mixed gradient analytic identifiers (from the id_analytic_gradients specification in RespGradMixed)

- IntSet idNumericalHessians
  mixed Hessian numerical identifiers (from the id_numerical_hessians specification in RespHessMixed)

- IntSet idQuasiHessians
  mixed Hessian quasi identifiers (from the id_quasi_hessians specification in RespHessMixed)

- IntSet idAnalyticHessians
  mixed Hessian analytic identifiers (from the id_analytic_hessians specification in RespHessMixed)

- IntVector fieldLengths
  number of entries in each field

- IntVector numCoordsPerField
  number of coordinates per field

- bool readFieldCoords
  Field data related storage: whether to read simulation field coordinates.

- StringArray varianceType
  Array which specifies the sigma type per response (none, one constant value, one per response (vector) or a full covariance matrix

Private Member Functions

- DataResponsesRep ()
  constructor

- ~DataResponsesRep ()
  destructor

  void write (std::ostream &s) const
  write a DataResponsesRep object to an std::ostream

  void read (MPIUnpackBuffer &s)
  read a DataResponsesRep object from a packed MPI buffer

  void write (MPIPackBuffer &s) const
  write a DataResponsesRep object to a packed MPI buffer

Private Attributes

- int referenceCount
  number of handle objects sharing this DataResponsesRep
CHAPTER 13. CLASS DOCUMENTATION

Friends

- class DataResponses
  
  *the handle class can access attributes of the body class directly*

13.36.1 Detailed Description

Body class for responses specification data.

The DataResponsesRep class is used to contain the data from a responses keyword specification. Default values are managed in the DataResponsesRep constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::dataResponsesList is private.

The documentation for this class was generated from the following files:

- DataResponses.hpp
- DataResponses.cpp

13.37 DataTransformModel Class Reference

Data transformation specialization of RecastModel.

Inheritance diagram for DataTransformModel:

```
Model

RecastModel

DataTransformModel
```

Public Member Functions

- DataTransformModel (const Model &sub_model, const ExperimentData &exp_data, size_t num_hyper=0, unsigned short multi_mode=CALIBRATE_NONE, short recast_resp_deriv_order=1)
  
  *standard constructor*

- ∼DataTransformModel ()
  
  *destructor*

- void data_transform_response (const Variables &sub_model_vars, const Response &sub_model_resp, Response &residual_resp)
  
  *Convenience function to help recover a residual response from the submodel.*

- void data_resize ()
  
  *The size of the ExperimentData changed; update the residualModel size.*

- void print_best_responses (std::ostream &s, const Variables &best_submodel_vars, const Response &best_submodel_resp, size_t num_best, size_t best_ind)
  
  *manage best responses including residuals and model responses per config*
Protected Types

- typedef std::map< int, IntResponseMap > IntIntResponseMapMap

Protected Member Functions

- void gen_primary_resp_map (const SharedResponseData &srd, Sizet2DArray &primary_resp_map_indices, BoolDequeArray &nonlinear_resp_map) const
  compute the primary response map for a data transform RecastModel
- void derived_evaluate (const ActiveSet &set)
  specialization of evaluate that iterates over configuration variables
- void derived_evaluate_nowait (const ActiveSet &set)
  specialization of evaluate that iterates over configuration variables
- const IntResponseMap & derived_synchronize ()
  synchronize all evaluations (all residuals for all experiment configurations)
- const IntResponseMap & derived_synchronize_nowait ()
  return any evaluations for which all experiment configurations have completed
- const IntResponseMap & filter_submodel_responses ()
- void cache_submodel_responses (const IntResponseMap &sm_resp_map, bool deep_copy)
  cache the subModel responses into a per-RecastModel eval ID map
- void collect_residuals (bool collect_all)
  collect any (or force all) completed subModel evals and populate recastResponseMap with residuals for those that
  are fully completed
- void transform_response_map (const IntResponseMap &submodel_resp, const Variables &recast_vars, Response &residual Resp)
  transform a set of per-configuration subModel Responses to a single evaluation’s residuals
- void scale_response (const Variables &submodel_vars, const Variables &recast_vars, Response &recast_response)
  scale the populated residual response by any covariance information, including hyper-parameter multipliers
- void init_continuous_vars ()
  Initialize continuous variable values/labels.
- template<typename T >
  void expand_array (const SharedResponseData &srd, const T &submodel_array, size_t recast_size, T &recast_array) const
  (if non-empty) expand submodel_array by replicates to populate a recast_array
- template<typename T >
  void expand_scales_array (const SharedResponseData &srd, const T &submodel_array, size_t submodel_array_size, size_t recast_size, T &recast_array) const
  If size greater than 1, expand submodel_array by replicates to populate a pre-sized recast_array, otherwise copy.
- void print_residual_response (const Response &residual_resp)
- void recover_submodel_responses (std::ostream &s, const Variables &best_submodel_vars, size_t num_best, best, size_t best_ind, Response &residual_resp)
Static Protected Member Functions

- static SizetArray variables_expand (const Model &sub_model, size_t num_hyper)
  expand the variable counts to account for hyper-parameters
- static int get_hyperparam_vc_index (const Model &sub_model)
  determine the index into vc_totals corresponding to where the hyper-parameters go
- static short response_order (const Model &sub_model, short recast_resp_order=1)
  helper to compute the recast response order during member initialization; recast_resp_order passed is the minimum request client needs
- static void vars_mapping (const Variables &recast_vars, Variables &submodel_vars)
  map the inbound expanded variables to the sub-model, discarding hyperparams (assumes hyper-parameters are at end of active continuous variables)
- static void set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)
  map the inbound ActiveSet to the sub-model (map derivative variables)
- static void primary_resp_differencer (const Variables &submodel_vars, const Variables &recast_vars, const Response &submodel_response, Response &recast_response)
  Recast callback function to difference residuals with observed data.

Protected Attributes

- const ExperimentData & expData
  Reference to the experiment data used to construct this Model.
- size_t numHyperparams
  Number of calibrated variance multipliers.
- unsigned short obsErrorMultiplierMode
  Calibration mode for the hyper-parameters.
- IntIntResponseMapMap cachedResp

Static Protected Attributes

- static DataTransformModel * dtModelInstance
  static pointer to this class for use in static callbacks

Additional Inherited Members

13.37.1 Detailed Description

Data transformation specialization of RecastModel.

Specialization of RecastModel to create a residual model that maps (1) from an augmented set of calibration parameters (including hyper-parameters) to those needed by the underlying simulation model and (2) from the simulation model response to a set of residuals, whose overall size may differ from the simulation (sub-model) response. The residuals may be scaled by experiment covariance information. This class provides a simple constructor that forwards to the more complicated RecastModel API.
13.37. **DATATRANSFORMMODEL CLASS REFERENCE**

### 13.37.2 Constructor & Destructor Documentation

**DataTransformModel (const Model & sub_model, const ExperimentData & exp_data, size_t num_hyper = 0, unsigned short mult_mode = CALIBRATE_NONE, short recast_resp_deriv_order = 1 )**

standard constructor

This constructor computes various indices and mappings, then updates the properties of the **RecastModel**. Hyper-parameters are assumed to trail the active continuous variables when presented to this **RecastModel**.

References Dakota::abort_handler(), Model::current_response(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), DataTransformModel::dtModelInstance, DataTransformModel::expand_array(), DataTransformModel::expand_scales_array(), DataTransformModel::expData, DataTransformModel::gen_primary_resp_map(), Model::icv(), Model::idiv(), Model::idrv(), Model::idsv(), Model::inactive_view(), DataTransformModel::init_continuous_vars(), RecastModel::init_maps(), ExperimentData::num_config_vars(), Model::num_primary_fns(), Model::num_secondary_fns(), ExperimentData::num_total_exppoints(), DataTransformModel::numHyperparams, DataTransformModel::primary_resp_differencer(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Model::primaryRespFnSense, Model::primaryRespFnWts, Model::scaling_options(), Model::scalingOpts, DataTransformModel::set_mapping(), Response::shared_data(), RecastModel::subModel, and DataTransformModel::vars_mapping().

### 13.37.3 Member Function Documentation

**SizeArray variables_expand (const Model & sub_model, size_t num_hyper ) [static], [protected]**

expand the variable counts to account for hyper-parameters

Incorporate the hyper parameters into Variables, assuming they are at the end of the active continuous variables. For example, append them to continuous design or continuous aleatory uncertain.

References SharedVariablesData::components_totals(), Model::current_variables(), DataTransformModel::get_hyperparam_vc_index(), Variables::shared_data(), and Dakota::svd().

**void derived_evaluate (const ActiveSet & set ) [protected], [virtual]**

specialization of evaluate that iterates over configuration variables

Blocking evaluation over all experiment configurations to compute a single set of expanded residuals. If the subModel supports asynchronous evaluate_nowait(), do the configuration evals concurrently and then synchronize.

Reimplemented from Model.

References Response::active_set(), Model::asynch_flag(), ExperimentData::config_vars(), Model::current_response(), Model::current_variables(), Model::currentResponse, Model::currentVariables, RecastModel::derived_evaluate(), Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), DataTransformModel::expData, DataTransformModel::filter_submodel_responses(), ExperimentData::form_residuals(), Model::inactive_variables(), ExperimentData::numperiments(), Model::outputLevel, RecastModel::recastIdMap, RecastModel::recastModelEvalCntr, DataTransformModel::scale_response(), RecastModel::subModel, DataTransformModel::transform_response_map(), RecastModel::transform_set(), and RecastModel::transform_variables().

**void derived_evaluate_nowait (const ActiveSet & set ) [protected], [virtual]**

specialization of evaluate that iterates over configuration variables

Non-blocking evaluation (scheduling) over all experiment configurations. Assumes that if this model supports nowait, its subModel does too and schedules them all.

Reimplemented from Model.
const IntResponseMap & derived_synchronize ( ) [protected], [virtual]

synchronize all evaluations (all residuals for all experiment configurations)

Collect all the subModel evaluations and build the residual sets for all evaluations. Like rekey functions in Dakota-Model, but many sub-model to one recast-model. For the blocking synchronize case, we force the subModel to sync and have all needed data.

Reimplemented from Model.
References DataTransformModel::cache_submodel_responses(), DataTransformModel::collect_residuals(), ExperimentData::config_vars(), RecastModel::derived_synchronize(), DataTransformModel::expData, RecastModel::recastResponseMap, RecastModel::subModel, and Model::synchronize().

const IntResponseMap & derived_synchronize_nowait ( ) [protected], [virtual]

return any evaluations for which all experiment configurations have completed

Collect any completed subModel evaluations and build the residual sets for any fully completed evaluations. Like rekey functions in DakotaModel, but many sub-model to one recast-model. We do not force the subModel to sync.

Reimplemented from Model.
References DataTransformModel::cache_submodel_responses(), DataTransformModel::collect_residuals(), ExperimentData::config_vars(), RecastModel::derived_synchronize_nowait(), DataTransformModel::expData, RecastModel::recastResponseMap, RecastModel::subModel, and Model::synchronize_nowait().

const IntResponseMap & filter_submodel_responses ( ) [protected]

(We don't quite want the rekey behavior since multiple subModel evaluations map to one recast eval.)

References Model::cache_unmatched_response(), RecastModel::recastIdMap, RecastModel::subModel, and Model::synchronize().

Referenced by DataTransformModel::derived_evaluate().

void transform_response_map ( const IntResponseMap & submodel Resp, const Variables & recast_vars, Response & residual Resp ) [protected]

transform a set of per-configuration subModel Responses to a single evaluation’s residuals

This transformation assumes the residuals are in submodel eval_id order.

References Dakota::abort_handler(), Model::current_variables(), DataTransformModel::expData, ExperimentData::form_residuals(), ExperimentData::num_experiments(), DataTransformModel::scale_response(), and RecastModel::subModel.

Referenced by DataTransformModel::collect_residuals(), and DataTransformModel::derived_evaluate().

void set_mapping ( const Variables & recast_vars, const ActiveSet & recast_set, ActiveSet & sub_model_set ) [static], [protected]

map the inbound ActiveSet to the sub-model (map derivative variables)

RecastModel sets up a default set mapping before calling this update, so focus on updating the derivative variables vector.
References Model::cv(), ActiveSet::derivative_vector(), DataTransformModel::dtModelInstance, DataTransformModel::numHyperparams, ActiveSet::request_vector(), and RecastModel::subordinate_model().

Referenced by DataTransformModel::DataTransformModel().

**void init_continuous_vars ( ) [protected]**

Initialize continuous variable values/labels.

Pull up the continuous variable values and labels into the RecastModel, inserting the hyper-parameter values/labels

References Model::all_continuous_variable(), Model::all_continuous_variable_label(), Model::all_continuous_variable_labels(), Model::all_continuous_variables(), SharedVariablesData::components_totals(), Model::current_variables(), DataTransformModel::expData, DataTransformModel::get_hyperparam_vc_index(), ExperimentData::hyperparam_labels(), DataTransformModel::numHyperparams, DataTransformModel::obsErrorMultiplierMode, Variables::shared_data(), RecastModel::subModel, and Dakota::svd().

Referenced by DataTransformModel::DataTransformModel().

**void expand_scales_array ( const SharedResponseData & srd, const T & submodel_array, size_t submodel_size, size_t recast_size, T & recast_array ) const [protected]**

If size greater than 1, expand submodel_array by replicates to populate a pre-sized recast_array, otherwise copy.

Passing the inbound array size so we can use one function for Teuchos and std containers (size vs. length)

References DataTransformModel::expand_array().

Referenced by DataTransformModel::DataTransformModel().

**13.38. DATAVARIABLES CLASS REFERENCE**

Handle class for variables specification data.

**Public Member Functions**

- **DataVariables ( )**
  
  *constructor*

- **DataVariables (const DataVariables &)**
  
  *copy constructor*

- **~DataVariables ( )**
  
  *destructor*
CHAPTER 13. CLASS DOCUMENTATION

- **DataVariables operator=** (const DataVariables &)
  
  assignment operator
- **bool operator==** (const DataVariables &)
  
  equality operator
- **void write**( std::ostream &s) const
  
  write a DataVariables object to an std::ostream
- **void read**( (MPIUnpackBuffer &s)
  
  read a DataVariables object from a packed MPI buffer
- **void write**( (MPIPackBuffer &s) const
  
  write a DataVariables object to a packed MPI buffer
- **DataVariablesRep * data_rep ()**
  
  return dataVarsRep
- **size_t design ()**
  
  return total number of design variables
- **size_t aleatory_uncertain ()**
  
  return total number of aleatory uncertain variables
- **size_t epistemic_uncertain ()**
  
  return total number of epistemic uncertain variables
- **size_t uncertain ()**
  
  return total number of uncertain variables
- **size_t state ()**
  
  return total number of state variables
- **size_t continuous_variables ()**
  
  return total number of continuous variables
- **size_t discrete_variables ()**
  
  return total number of discrete variables
- **size_t total_variables ()**
  
  return total number of variables

**Static Public Member Functions**

- **static bool id_compare** (const DataVariables &dv, const std::string &id)
  
  compares the idVariables attribute of DataVariables objects

**Private Attributes**

- **DataVariablesRep * dataVarsRep**
  
  pointer to the body (handle-body idiom)

**Friends**

- class ProblemDescDB
- class NIDRProblemDescDB
13.38.1 Detailed Description

Handle class for variables specification data.

The DataVariables class is used to provide a memory management handle for the data in DataVariablesRep. It is populated by IDRProblemDescDB::variables_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataVariables objects is maintained in ProblemDescDB::dataVariablesList, one for each variables specification in an input file.

The documentation for this class was generated from the following files:

- DataVariables.hpp
- DataVariables.cpp

13.39 DataVariablesRep Class Reference

Body class for variables specification data.

Public Attributes

- String idVariables
  string identifier for the variables specification data set (from the id_variables specification in VarSetId)
- short varsView
  user selection/override of variables view: {DEFAULT,ALL,DESIGN,UNCERTAIN,ALEATORY,UNCERTAIN,EPISTEMIC,UNCERTAIN,STATE}_VIEW
- short varsDomain
  user selection/override of variables domain: {DEFAULT,MIXED,RELAXED}_DOMAIN
- bool uncertainVarsInitPt
  flag indicating user specification of initial points (for local optimization-based UQ methods) for at least one uncertain variable type
- size_t numContinuousDesVars
  number of continuous design variables (from the continuous_design specification in VarDV)
- size_t numDiscreteDesRangeVars
  number of discrete design variables defined by an integer range (from the discrete_design_range specification in VarDV)
- size_t numDiscreteDesSetIntVars
  number of discrete design variables defined by a set of integers (from the discrete_design_set integer specification in VarDV)
- size_t numDiscreteDesSetStrVars
  number of discrete design variables defined by a set of strings (from the discrete_design_set string specification in VarDV)
- size_t numDiscreteDesSetRealVars
  number of discrete design variables defined by a set of reals (from the discrete_design_set real specification in VarDV)
- size_t numNormalUncVars
  number of normal uncertain variables (from the normal_uncertain specification in VarAUV)
- size_t numLognormalUncVars
  number of lognormal uncertain variables (from the lognormal_uncertain specification in VarAUV)
- size_t numUniformUncVars
number of uniform uncertain variables (from the uniform_uncertain specification in VarAUV)

- `size_t numLoguniformUncVars`
  number of loguniform uncertain variables (from the loguniform_uncertain specification in VarAUV)

- `size_t numTriangularUncVars`
  number of triangular uncertain variables (from the triangular_uncertain specification in VarAUV)

- `size_t numExponentialUncVars`
  number of exponential uncertain variables (from the exponential_uncertain specification in VarAUV)

- `size_t numBetaUncVars`
  number of beta uncertain variables (from the beta_uncertain specification in VarAUV)

- `size_t numGammaUncVars`
  number of gamma uncertain variables (from the gamma_uncertain specification in VarAUV)

- `size_t numGumbelUncVars`
  number of gumbel uncertain variables (from the gumbel_uncertain specification in VarAUV)

- `size_t numFrechetUncVars`
  number of frechet uncertain variables (from the frechet_uncertain specification in VarAUV)

- `size_t numWeibullUncVars`
  number of weibull uncertain variables (from the weibull_uncertain specification in VarAUV)

- `size_t numHistogramBinUncVars`
  number of histogram bin uncertain variables (from the histogram_bin_uncertain specification in VarAUV)

- `size_t numPoissonUncVars`
  number of Poisson uncertain variables (from the poisson_uncertain specification in VarAUV)

- `size_t numBinomialUncVars`
  number of binomial uncertain variables (from the binomial_uncertain specification in VarAUV)

- `size_t numNegBinomialUncVars`
  number of negative binomial uncertain variables (from the negative_binomial_uncertain specification in VarAUV)

- `size_t numGeometricUncVars`
  number of geometric uncertain variables (from the geometric_uncertain specification in VarAUV)

- `size_t numHyperGeomUncVars`
  number of hypergeometric uncertain variables (from the hypergeometric_uncertain specification in VarAUV)

- `size_t numHistogramPtIntUncVars`
  number of integer-valued histogram point uncertain variables (from the histogram_point_uncertain specification in VarAUV)

- `size_t numHistogramPtStrUncVars`
  number of string-valued histogram point uncertain variables (from the histogram_point_uncertain specification in VarAUV)

- `size_t numHistogramPtRealUncVars`
  number of real-valued histogram point uncertain variables (from the histogram_point_uncertain specification in VarAUV)

- `size_t numContinuousIntervalUncVars`
  number of continuous epistemic interval uncertain variables (from the continuous_interval_uncertain specification in VarEUV)

- `size_t numDiscreteIntervalUncVars`
number of discrete epistemic interval uncertain variables (from the `discrete_interval_uncertain` specification in VarEUV)

- `size_t numDiscreteUncSetIntVars`
  number of discrete epistemic uncertain integer set variables (from the `discrete_uncertain_set integer` specification in VarEUV)

- `size_t numDiscreteUncSetStrVars`
  number of discrete epistemic uncertain string set variables (from the `discrete_uncertain_set string` specification in VarEUV)

- `size_t numDiscreteUncSetRealVars`
  number of discrete epistemic uncertain real set variables (from the `discrete_uncertain_set real` specification in VarEUV)

- `size_t numContinuousStateVars`
  number of continuous state variables (from the `continuous_state` specification in VarSV)

- `size_t numDiscreteStateRangeVars`
  number of discrete state variables defined by an integer range (from the `discrete_state_range` specification in VarDV)

- `size_t numDiscreteStateSetIntVars`
  number of discrete state variables defined by a set of integers (from the `discrete_state_set integer` specification in VarDV)

- `size_t numDiscreteStateSetStrVars`
  number of discrete state variables defined by a set of strings (from the `discrete_state_set string` specification in VarDV)

- `size_t numDiscreteStateSetRealVars`
  number of discrete state variables defined by a set of reals (from the `discrete_state_set real` specification in VarDV)

- `RealVector continuousDesignVars`
  initial values for the continuous design variables array (from the `continuous_design initial_point` specification in VarDV)

- `RealVector continuousDesignLowerBnds`
  lower bounds array for the continuous design variables (from the `continuous_design lower_bounds` specification in VarDV)

- `RealVector continuousDesignUpperBnds`
  upper bounds array for the continuous design variables (from the `continuous_design upper_bounds` specification in VarDV)

- `StringArray continuousDesignScaleTypes`
  scale types array for the continuous design variables (from the `continuous_design scale_types` specification in VarDV)

- `RealVector continuousDesignScales`
  scales array for the continuous design variables (from the `continuous_design scales` specification in VarDV)

- `IntVector discreteDesignRangeVars`
  initial values for the discrete design variables defined by an integer range (from the `discrete_design_range initial_point` specification in VarDV)

- `IntVector discreteDesignRangeLowerBnds`
  lower bounds array for the discrete design variables defined by an integer range (from the `discrete_design_range lower_bounds` specification in VarDV)
• **IntVector** `discreteDesignRangeUpperBnds`
  > upper bounds array for the discrete design variables defined by an integer range (from the `discrete_design_range_upper_bounds` specification in VarDV)
• **BitArray** `discreteDesignRangeCat`
  > is each ddr var strictly categorical (true) or relaxable (false)
• **IntVector** `discreteDesignSetIntVars`
  > initial values for the discrete design variables defined by an integer set (from the `discrete_design_set integer initial_point` specification in VarDV)
• **StringArray** `discreteDesignSetStrVars`
  > initial values for the discrete design variables defined by a string set (from the `discrete_design_set string initial_point` specification in VarDV)
• **RealVector** `discreteDesignSetRealVars`
  > initial values for the discrete design variables defined by a real set (from the `discrete_design_set real initial_point` specification in VarDV)
• **IntSetArray** `discreteDesignSetInt`
  > complete set of admissible values for each of the discrete design variables defined by an integer set (from the `discrete_design_set integer set_values` specification in VarDV)
• **StringSetArray** `discreteDesignSetStr`
  > complete set of admissible values for each of the discrete design variables defined by a string set (from the `discrete_design_set string set_values` specification in VarDV)
• **RealSetArray** `discreteDesignSetReal`
  > complete set of admissible values for each of the discrete design variables defined by a real set (from the `discrete_design_set real set_values` specification in VarDV)
• **BitArray** `discreteDesignSetIntCat`
  > is each ddsi var strictly categorical (true) or relaxable (false)
• **BitArray** `discreteDesignSetRealCat`
  > is each ddsr var strictly categorical (true) or relaxable (false)
• **RealMatrixArray** `discreteDesignSetIntAdj`
  > Adjacency matrices for each of the discrete design variables defined by an integer set (from the `discrete_design_set integer categorical adjacency` specification in VarDV)
• **RealMatrixArray** `discreteDesignSetStrAdj`
  > Adjacency matrices for each of the discrete design variables defined by a string set (from the `discrete_design_set string adjacency` specification in VarDV)
• **RealMatrixArray** `discreteDesignSetRealAdj`
  > Adjacency matrices for each of the discrete design variables defined by a real set (from the `discrete_design_set real categorical adjacency` specification in VarDV)
• **StringArray** `continuousDesignLabels`
  > labels array for the continuous design variables (from the `continuous_design descriptors` specification in VarDV)
• **StringArray** `discreteDesignRangeLabels`
  > labels array for the discrete design variables defined by an integer range (from the `discrete_design_range descriptors` specification in VarDV)
• **StringArray** `discreteDesignSetIntLabels`
  > labels array for the discrete design variables defined by an integer set (from the `discrete_design_set int descriptors` specification in VarDV)
• **StringArray** `discreteDesignSetStrLabels`
labels array for the discrete design variables defined by a string set (from the \texttt{discrete\_design\_set} string descriptors specification in VarDV)

- StringArray \texttt{discrete\_Design\_Set\_Real\_Labels}
  
  labels array for the discrete design variables defined by a real set (from the \texttt{discrete\_design\_set} real; descriptors specification in VarDV)

- RealVector \texttt{normal\_Unc\_Means}
  
  means of the normal uncertain variables (from the \texttt{means} specification in VarCAUV\_Normal)

- RealVector \texttt{normal\_Unc\_Std\_Devs}
  
  standard deviations of the normal uncertain variables (from the \texttt{std\_deviations} specification in VarCAUV\_Normal)

- RealVector \texttt{normal\_Unc\_Lower\_Bnds}
  
  distribution lower bounds for the normal uncertain variables (from the \texttt{lower\_bounds} specification in VarCAUV\_Normal)

- RealVector \texttt{normal\_Unc\_Upper\_Bnds}
  
  distribution upper bounds for the normal uncertain variables (from the \texttt{upper\_bounds} specification in VarCAUV\_Normal)

- RealVector \texttt{normal\_Unc\_Vars}
  
  initial values of the normal uncertain variables (from the \texttt{initial\_point} specification in VarCAUV\_Normal)

- RealVector \texttt{lognormal\_Unc\_Lambdas}
  
  \texttt{lambdas} (means of the corresponding normals) of the lognormal uncertain variables (from the \texttt{lambdas} specification in VarCAUV\_Lognormal)

- RealVector \texttt{lognormal\_Unc\_Zetas}
  
  \texttt{zetas} (standard deviations of the corresponding normals) of the lognormal uncertain variables (from the \texttt{zetas} specification in VarCAUV\_Lognormal)

- RealVector \texttt{lognormal\_Unc\_Means}
  
  means of the lognormal uncertain variables (from the \texttt{means} specification in VarCAUV\_Lognormal)

- RealVector \texttt{lognormal\_Unc\_Std\_Devs}
  
  standard deviations of the lognormal uncertain variables (from the \texttt{std\_deviations} specification in VarCAUV\_Lognormal)

- RealVector \texttt{lognormal\_Unc\_Err\_Facts}
  
  error factors for the lognormal uncertain variables (from the \texttt{error\_factors} specification in VarCAUV\_Lognormal)

- RealVector \texttt{lognormal\_Unc\_Lower\_Bnds}
  
  distribution lower bounds for the lognormal uncertain variables (from the \texttt{lower\_bounds} specification in VarCAUV\_Lognormal)

- RealVector \texttt{lognormal\_Unc\_Upper\_Bnds}
  
  distribution upper bounds for the lognormal uncertain variables (from the \texttt{upper\_bounds} specification in VarCAUV\_Lognormal)

- RealVector \texttt{lognormal\_Unc\_Vars}
  
  initial values of the lognormal uncertain variables (from the \texttt{initial\_point} specification in VarCAUV\_Lognormal)

- RealVector \texttt{uniform\_Unc\_Lower\_Bnds}
  
  distribution lower bounds for the uniform uncertain variables (from the \texttt{lower\_bounds} specification in VarCAUV\_Uniform)

- RealVector \texttt{uniform\_Unc\_Upper\_Bnds}
  
  distribution upper bounds for the uniform uncertain variables (from the \texttt{upper\_bounds} specification in VarCAUV\_Uniform)
• RealVector `uniformUncVars`
  initial values of the uniform uncertain variables (from the initial_point specification in VarCAUV_Uniform)
• RealVector `loguniformUncLowerBnds`
  distribution lower bounds for the loguniform uncertain variables (from the lower_bounds specification in VarCAUV_Loguniform)
• RealVector `loguniformUncUpperBnds`
  distribution upper bounds for the loguniform uncertain variables (from the upper_bounds specification in VarCAUV_Loguniform)
• RealVector `loguniformUncVars`
  initial values of the loguniform uncertain variables (from the initial_point specification in VarCAUV_Loguniform)
• RealVector `triangularUncModes`
  modes of the triangular uncertain variables (from the modes specification in VarCAUV_Triangular)
• RealVector `triangularUncLowerBnds`
  distribution lower bounds for the triangular uncertain variables (from the lower_bounds specification in VarCAUV_Triangular)
• RealVector `triangularUncUpperBnds`
  distribution upper bounds for the triangular uncertain variables (from the upper_bounds specification in VarCAUV_Triangular)
• RealVector `triangularUncVars`
  initial values of the triangular uncertain variables (from the initial_point specification in VarCAUV_Triangular)
• RealVector `exponentialUncBetas`
  beta factors for the exponential uncertain variables (from the betas specification in VarCAUV_Exponential)
• RealVector `exponentialUncVars`
  initial values of the exponential uncertain variables (from the initial_point specification in VarCAUV_Exponential)
• RealVector `betaUncAlphas`
  alpha factors for the beta uncertain variables (from the means specification in VarCAUV_Beta)
• RealVector `betaUncBetas`
  beta factors for the beta uncertain variables (from the std_deviations specification in VarCAUV_Beta)
• RealVector `betaUncLowerBnds`
  distribution lower bounds for the beta uncertain variables (from the lower_bounds specification in VarCAUV_Beta)
• RealVector `betaUncUpperBnds`
  distribution upper bounds for the beta uncertain variables (from the upper_bounds specification in VarCAUV_Beta)
• RealVector `betaUncVars`
  initial values of the beta uncertain variables (from the initial_point specification in VarCAUV_Beta)
• RealVector `gammaUncAlphas`
  alpha factors for the gamma uncertain variables (from the alphas specification in VarCAUV_Gamma)
• RealVector `gammaUncBetas`
  beta factors for the gamma uncertain variables (from the betas specification in VarCAUV_Gamma)
• RealVector `gammaUncVars`
  initial values of the gamma uncertain variables (from the initial_point specification in VarCAUV_Gamma)
• RealVector `gumbelUncAlphas`
alpha factors for the gumbel uncertain variables (from the alphas specification in VarCAUV_Gumbel)
• RealVector gumbelUncBetas
  beta factors for of the gumbel uncertain variables (from the betas specification in VarCAUV_Gumbel)
• RealVector gumbelUncVars
  initial values of the gumbel uncertain variables (from the initial_point specification in VarCAUV_Gumbel)
• RealVector frechetUncAlphas
  alpha factors for the frechet uncertain variables (from the alphas specification in VarCAUV_Frechet)
• RealVector frechetUncBetas
  beta factors for the frechet uncertain variables (from the betas specification in VarCAUV_Frechet)
• RealVector frechetUncVars
  initial values of the frechet uncertain variables (from the initial_point specification in VarCAUV_Frechet)
• RealVector weibullUncAlphas
  alpha factors for the weibull uncertain variables (from the alphas specification in VarCAUV_Weibull)
• RealVector weibullUncBetas
  beta factors for the weibull uncertain variables (from the betas specification in VarCAUV_Weibull)
• RealVector weibullUncVars
  initial values of the weibull uncertain variables (from the initial_point specification in VarCAUV_Weibull)
• RealRealMapArray histogramUncBinPairs
  An array for each real-valued bin-based histogram uncertain variable. Each array entry is a map from a real value to its probability. (See continuous linear histogram in LHS manual; from the histogram.bin.uncertain specification in VarCAUV_Bin_Histogram). (x,y) ordinate specifications are converted to (x,c) counts within NIDR.
• RealVector histogramBinUncVars
  initial values of the histogram bin uncertain variables (from the initial_point specification in VarCAUV_Bin_Histogram)
• RealVector poissonUncLambdas
  lambdas (rate parameter) for the poisson uncertain variables (from the lambdas specification in VarDAUV_Poisson)
• IntVector poissonUncVars
  initial values of the poisson uncertain variables (from the initial_point specification in VarDAUV_Poisson)
• BitArray poissonUncCat
  is each poisson var strictly categorical (true) or relaxable (false)
• RealVector binomialUncProbPerTrial
  probabilities per each trial (p) for the binomial uncertain variables from the prob_per_trial specification in VarDAUV_Binomial)
• IntVector binomialUncNumTrials
  Number of trials (N) for the binomial uncertain variables from the num_trials specification in VarDAUV_Binomial)
• IntVector binomialUncVars
  initial values of the binomial uncertain variables (from the initial_point specification in VarDAUV_Binomial)
• BitArray binomialUncCat
  is each binomial var strictly categorical (true) or relaxable (false)
• RealVector negBinomialUncProbPerTrial
  probabilities per each trial (p) for the negative binomial uncertain variables from the prob_per_trial specification in VarDAUV_Negative_Binomial)
- IntVector negBinomialUncNumTrials
  Number of trials (N) for the negative binomial uncertain variables from the num_trials specification in VarDAUV_Negative_Binomial

- IntVector negBinomialUncVars
  initial values of the negative binomial uncertain variables (from the initial_point specification in VarDAUV_Negative_Binomial)

- BitArray negBinomialUncCat
  is each negbinomial var strictly categorical (true) or relaxable (false)

- RealVector geometricUncProbPerTrial
  probabilities per each trial (p) for the geometric uncertain variables from the prob_per_trial specification in VarDAUV_Geometric

- IntVector geometricUncVars
  initial values of the geometric uncertain variables (from the initial_point specification in VarDAUV_Geometric)

- BitArray geometricUncCat
  is each geometric var strictly categorical (true) or relaxable (false)

- IntVector hyperGeomUncTotalPop
  Size of total populations (N) for the hypergeometric uncertain variables from the total_population specification in VarDAUV_Hypergeometric

- IntVector hyperGeomUncSelectedPop
  Size of selected populations for the hypergeometric uncertain variables from the selected_population specification in VarDAUV_Hypergeometric

- IntVector hyperGeomUncNumDrawn
  Number failed in the selected populations for the hypergeometric variables from the num_drawn specification in VarDAUV_Hypergeometric

- IntVector hyperGeomUncVars
  initial values of the hypergeometric uncertain variables (from the initial_point specification in VarDAUV_Hypergeometric)

- BitArray hyperGeomUncCat
  is each hypergeom var strictly categorical (true) or relaxable (false)

- IntRealMapArray histogramUncPointIntPairs
  An array for each integer-valued point-based histogram uncertain variable. Each array entry is a map from an integer value to its probability. (See discrete histogram in LHS manual; from the histogram_point_uncertain specification in VarDAUV_Point_Histogram)

- IntVector histogramUncPointIntVars
  initial values of the real-valued histogram point uncertain variables (from the initial_point specification in VarDAUV_Point_Histogram)

- BitArray histogramUncPointIntCat
  is each hupi var strictly categorical (true) or relaxable (false)

- StringRealMapArray histogramUncPointStrPairs
  An array for each string-valued point-based histogram uncertain variable. Each array entry is a map from a string value to its probability. (See discrete histogram in LHS manual; from the histogram_point_uncertain specification in VarDAUV_Point_Histogram)

- StringArray histogramUncPointStrUncVars
  initial values of the real-valued histogram point uncertain variables (from the initial_point specification in VarDAUV_Point_Histogram)

- RealRealMapArray histogramUncPointRealPairs
An array for each real-valued point-based histogram uncertain variable. Each array entry is a map from a real value to its probability. (See discrete histogram in LHS manual; from the histogram_point_uncertain specification in VarDAUV_Point_Histogram)

- **RealVector** histogramPointRealUncVars
  initial values of the real-valued histogram point uncertain variables (from the initial_point specification in VarDAUV_Point_Histogram)

- **BitArray** histogramUncPointRealCat
  is each hupr var strictly categorical (true) or relaxable (false)

- **RealSymMatrix** uncertainCorrelations
  correlation matrix for all uncertain variables (from the uncertain_correlation_matrix specification in VarAUV_Correlations). This matrix specifies rank correlations for LHS sampling and correlation coefficients ($\rho_{ij} =$ normalized covariance matrix) for other methods.

- **RealRealPairRealMapArray** continuousIntervalUncBasicProbs
  Probability values per interval cell per epistemic interval uncertain variable (from the continuous_interval_uncertain_interval_probs specification in VarCEUV_Interval)

- **RealVector** continuousIntervalUncVars
  initial values of the continuous interval uncertain variables (from the initial_point specification in VarCEUV_Interval)

- **IntIntPairRealMapArray** discreteIntervalUncBasicProbs
  Probability values per interval cell per epistemic interval uncertain variable (from the discrete_interval_uncertain_interval_probs specification in VarDIUV)

- **IntVector** discreteIntervalUncVars
  initial values of the discrete interval uncertain variables (from the initial_point specification in VarDIUV)

- **BitArray** discreteIntervalUncCat
  is each diu var strictly categorical (true) or relaxable (false)

- **IntRealMapArray** discreteUncSetIntValuesProbs
  complete set of admissible values with associated basic probability assignments for each of the discrete epistemic uncertain variables defined by an integer set (from the discrete_uncertain_set_integer_set_values specification in VarDUSIV)

- **IntVector** discreteUncSetIntVars
  initial values of the discrete uncertain set integer variables (from the initial_point specification in VarDUSIV)

- **BitArray** discreteUncSetIntCat
  is each dusi var strictly categorical (true) or relaxable (false)

- **StringRealMapArray** discreteUncSetStrValuesProbs
  complete set of admissible values with associated basic probability assignments for each of the discrete epistemic uncertain variables defined by a string set (from the discrete_uncertain_set_string_set_values specification in VarDUSIV)

- **StringArray** discreteUncSetStrVars
  initial values of the discrete uncertain set integer variables (from the initial_point specification in VarDUSIV)

- **RealRealMapArray** discreteUncSetRealValuesProbs
  complete set of admissible values with associated basic probability assignments for each of the discrete epistemic uncertain variables defined by a real set (from the discrete_uncertain_set_real_set_values specification in VarDUSRV)

- **RealVector** discreteUncSetRealVars
  initial values of the discrete uncertain set real variables (from the initial_point specification in VarDUSRV)

- **BitArray** discreteUncSetRealCat
is each dsr var strictly categorical (true) or relaxable (false)

- **RealVector** `continuousStateVars`  
  initial values for the continuous state variables array (from the `continuous_state_initial_point` specification in VarSV)

- **RealVector** `continuousStateLowerBnds`  
  lower bounds array for the continuous state variables (from the `continuous_state_lower_bounds` specification in VarSV)

- **RealVector** `continuousStateUpperBnds`  
  upper bounds array for the continuous state variables (from the `continuous_state_upper_bounds` specification in VarSV)

- **IntVector** `discreteStateRangeVars`  
  initial values for the discrete state variables defined by an integer range (from the `discrete_state_range_initial_point` specification in VarSV)

- **IntVector** `discreteStateRangeLowerBnds`  
  lower bounds array for the discrete state variables defined by an integer range (from the `discrete_state_range_lower_bounds` specification in VarSV)

- **IntVector** `discreteStateRangeUpperBnds`  
  upper bounds array for the discrete state variables defined by an integer range (from the `discrete_state_range_upper_bounds` specification in VarSV)

- **BitArray** `discreteStateRangeCat`  
  is each dsr var strictly categorical (true) or relaxable (false)

- **IntVector** `discreteStateSetIntVars`  
  initial values for the discrete state variables defined by an integer set (from the `discrete_state_set_integer_initial_point` specification in VarSV)

- **StringArray** `discreteStateSetStrVars`  
  initial values for the discrete state variables defined by a string set (from the `discrete_state_set_string_initial_point` specification in VarSV)

- **RealVector** `discreteStateSetRealVars`  
  initial values for the discrete state variables defined by a real set (from the `discrete_state_set_real_initial_point` specification in VarSV)

- **IntSetArray** `discreteStateSetInt`  
  complete set of admissible values for each of the discrete state variables defined by an integer set (from the `discrete_state_set_integer_set_values` specification in VarSV)

- **StringSetArray** `discreteStateSetStr`  
  complete set of admissible values for each of the discrete state variables defined by a string set (from the `discrete_state_set_string_set_values` specification in VarSV)

- **RealSetArray** `discreteStateSetReal`  
  complete set of admissible values for each of the discrete state variables defined by a real set (from the `discrete_state_set_real_set_values` specification in VarSV)

- **BitArray** `discreteStateSetIntCat`  
  is each dssi var strictly categorical (true) or relaxable (false)

- **BitArray** `discreteStateSetRealCat`  
  is each dsr var strictly categorical (true) or relaxable (false)

- **StringArray** `continuousStateLabels`  
  labels array for the continuous state variables (from the `continuous_state_descriptors` specification in VarSV)
• StringArray discreteStateRangeLabels
  labels array for the discrete state variables defined by an integer range (from the discrete state range
  descriptors specification in VarSV)
• StringArray discreteStateSetIntLabels
  labels array for the discrete state variables defined by an integer set (from the discrete state set descriptors
  specification in VarSV)
• StringArray discreteStateSetStrLabels
  labels array for the discrete state variables defined by a string set (from the discrete state set descriptors
  specification in VarSV)
• StringArray discreteStateSetRealLabels
  labels array for the discrete state variables defined by a real set (from the discrete state set descriptors
  specification in VarSV)
• IntVector discreteDesignSetIntLowerBnds
  discrete design integer set lower bounds inferred from set values
• IntVector discreteDesignSetIntUpperBnds
  discrete design integer set upper bounds inferred from set values
• StringArray discreteDesignSetStrLowerBnds
  discrete design string set lower bounds inferred from set values
• StringArray discreteDesignSetStrUpperBnds
  discrete design string set upper bounds inferred from set values
• RealVector discreteDesignSetRealLowerBnds
  discrete design real set lower bounds inferred from set values
• RealVector discreteDesignSetRealUpperBnds
  discrete design real set upper bounds inferred from set values
• RealVector continuousAleatoryUncVars
  array of values for all continuous aleatory uncertain variables
• RealVector continuousAleatoryUncLowerBnds
  distribution lower bounds for all continuous aleatory uncertain variables (collected from nuv_lower_bounds,
  lnuv_lower_bounds, uuv_lower_bounds, luuv_lower_bounds, tvu_lower_bounds, and buv_lower_bounds specifications in VarAUV,
  and derived for gamma, gumbel, frechet, weibull and histogram bin specifications)
• RealVector continuousAleatoryUncUpperBnds
  distribution upper bounds for all continuous aleatory uncertain variables (collected from nuv_upper_bounds,
  lnuv_upper_bounds, uuv_upper_bounds, luuv_upper_bounds, tvu_lower_bounds, and buv_upper_bounds specifications in VarAUV,
  and derived for gamma, gumbel, frechet, weibull and histogram bin specifications)
• StringArray continuousAleatoryUncLabels
  labels for all continuous aleatory uncertain variables (collected from nuv_descriptors, lnuv_descriptors,
  uuv_descriptors, luuv_descriptors, tvu_descriptors, buv_descriptors, gauv_descriptors, guuv_descriptors,
  fuv_descriptors, wuv_descriptors, and hbuv_descriptors specifications in VarAUV)
• IntVector discreteIntAleatoryUncVars
  array of values for all discrete integer aleatory uncertain variables
• IntVector discreteIntAleatoryUncLowerBnds
  distribution lower bounds for all discrete integer aleatory uncertain variables
• IntVector discreteIntAleatoryUncUpperBnds
distribution upper bounds for all discrete integer aleatory uncertain variables
- **StringArray** `discreteIntAleatoryUncLabels`  
  labels for all discrete integer aleatory uncertain variables
- **StringArray** `discreteStrAleatoryUncVars`  
  array of values for all discrete string epistemic uncertain variables
- **StringArray** `discreteStrAleatoryUncLowerBnds`  
  distribution lower bounds for all discrete string epistemic uncertain variables
- **StringArray** `discreteStrAleatoryUncUpperBnds`  
  distribution upper bounds for all discrete string epistemic uncertain variables
- **StringArray** `discreteStrAleatoryUncLabels`  
  labels for all discrete string epistemic uncertain variables
- **RealVector** `discreteRealAleatoryUncVars`  
  array of values for all discrete real aleatory uncertain variables
- **RealVector** `discreteRealAleatoryUncLowerBnds`  
  distribution lower bounds for all discrete real aleatory uncertain variables
- **RealVector** `discreteRealAleatoryUncUpperBnds`  
  distribution upper bounds for all discrete real aleatory uncertain variables
- **StringArray** `discreteRealAleatoryUncLabels`  
  labels for all discrete real aleatory uncertain variables
- **RealVector** `continuousEpistemicUncVars`  
  array of values for all continuous epistemic uncertain variables
- **RealVector** `continuousEpistemicUncLowerBnds`  
  distribution lower bounds for all continuous epistemic uncertain variables
- **RealVector** `continuousEpistemicUncUpperBnds`  
  distribution upper bounds for all continuous epistemic uncertain variables
- **StringArray** `continuousEpistemicUncLabels`  
  labels for all continuous epistemic uncertain variables
- **IntVector** `discreteIntEpistemicUncVars`  
  array of values for all discrete integer epistemic uncertain variables
- **IntVector** `discreteIntEpistemicUncLowerBnds`  
  distribution lower bounds for all discrete integer epistemic uncertain variables
- **IntVector** `discreteIntEpistemicUncUpperBnds`  
  distribution upper bounds for all discrete integer epistemic uncertain variables
- **StringArray** `discreteIntEpistemicUncLabels`  
  labels for all discrete integer epistemic uncertain variables
- **StringArray** `discreteStrEpistemicUncVars`  
  array of values for all discrete string epistemic uncertain variables
- **StringArray** `discreteStrEpistemicUncLowerBnds`  
  distribution lower bounds for all discrete string epistemic uncertain variables
- **StringArray** `discreteStrEpistemicUncUpperBnds`  
  distribution upper bounds for all discrete string epistemic uncertain variables
- **StringArray** `discreteStrEpistemicUncLabels`  
  labels for all discrete string epistemic uncertain variables
- RealVector `discreteRealEpistemicUncVars`
  array of values for all discrete real epistemic uncertain variables
- RealVector `discreteRealEpistemicUncLowerBnds`
  distribution lower bounds for all discrete real epistemic uncertain variables
- RealVector `discreteRealEpistemicUncUpperBnds`
  distribution upper bounds for all discrete real epistemic uncertain variables
- StringArray `discreteRealEpistemicUncLabels`
  labels for all discrete real epistemic uncertain variables
- IntVector `discreteStateSetIntLowerBnds`
  discrete state integer set lower bounds inferred from set values
- IntVector `discreteStateSetIntUpperBnds`
  discrete state integer set upper bounds inferred from set values
- StringArray `discreteStateSetStrLowerBnds`
  discrete state string set lower bounds inferred from set values
- StringArray `discreteStateSetStrUpperBnds`
  discrete state string set upper bounds inferred from set values
- RealVector `discreteStateSetRealLowerBnds`
  discrete state real set lower bounds inferred from set values
- RealVector `discreteStateSetRealUpperBnds`
  discrete state real set upper bounds inferred from set values
- RealVector `linearIneqConstraintCoeffs`
  coefficient matrix for the linear inequality constraints (from the `linear_inequality_constraint_matrix` specification in MethodIndControl)
- RealVector `linearIneqLowerBnds`
  lower bounds for the linear inequality constraints (from the `linear_inequality_lower_bounds` specification in MethodIndControl)
- RealVector `linearIneqUpperBnds`
  upper bounds for the linear inequality constraints (from the `linear_inequality_upper_bounds` specification in MethodIndControl)
- StringArray `linearIneqScaleTypes`
  scaling types for the linear inequality constraints (from the `linear_inequality_scale_types` specification in MethodIndControl)
- RealVector `linearIneqScales`
  scaling factors for the linear inequality constraints (from the `linear_inequality_scales` specification in MethodIndControl)
- RealVector `linearEqConstraintCoeffs`
  coefficient matrix for the linear equality constraints (from the `linear_equality_constraint_matrix` specification in MethodIndControl)
- RealVector `linearEqTargets`
  targets for the linear equality constraints (from the `linear_equality_targets` specification in MethodIndControl)
- StringArray `linearEqScaleTypes`
  scaling types for the linear equality constraints (from the `linear_equality_scale_types` specification in MethodIndControl)
- RealVector `linearEqScales`
  scaling factors for the linear equality constraints (from the `linear_equality_scales` specification in MethodIndControl)
Private Member Functions

- **DataVariablesRep ()**
  - default constructor
- **~DataVariablesRep ()**
  - destructor
- **void write (std::ostream &s) const**
  - write a DataVariablesRep object to an std::ostream
- **void read (MPIUnpackBuffer &s)**
  - read a DataVariablesRep object from a packed MPI buffer
- **void write (MPIPackBuffer &s) const**
  - write a DataVariablesRep object to a packed MPI buffer

Private Attributes

- **int referenceCount**
  - number of handle objects sharing dataVarsRep

Friends

- **class DataVariables**
  - the handle class can access attributes of the body class directly

13.39.1 Detailed Description

Body class for variables specification data.

The `DataVariablesRep` class is used to contain the data from a variables keyword specification. Default values are managed in the `DataVariablesRep` constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within `ProblemDescDB` since `ProblemDescDB::dataVariablesList` is private.

The documentation for this class was generated from the following files:

- DataVariables.hpp
- DataVariables.cpp

13.40 DDACEDesignCompExp Class Reference

Wrapper class for the DDACE design of experiments library.

Inheritance diagram for DDACEDesignCompExp:

```
          Iterator
           |
          Analyzer
           |
PStudyDACE
           |
DDACEDesignCompExp
```
Public Member Functions

- `DDACEDesignCompExp (ProblemDescDB &problem_db, Model &model)`
  primary constructor for building a standard DACE iterator
- `DDACEDesignCompExp (Model &model, int samples, int symbols, int seed, unsigned short sampling_method)`
  alternate constructor used for building approximations
- `~DDACEDesignCompExp ()`
  destructor
- `bool resize ()`
  reinitializes iterator based on new variable size

Protected Member Functions

- `void pre_run ()`
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- `void core_run ()`
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- `void post_input ()`
  read tabular data for post-run mode
- `void post_run (std::ostream &s)`
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
- `int num_samples () const`
  reset sampling iterator to use at least min_samples
- `void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)`
  reset sampling iterator to use at least min_samples
- `unsigned short sampling_scheme () const`
  return sampling name
- `void vary_pattern (bool pattern_flag)`
  sets varyPattern in derived classes that support it
- `void get_parameter_sets (Model &model)`
  Generate one block of numSamples samples (ndim * num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
- `void get_parameter_sets (Model &model, const int num_samples, RealMatrix &design_matrix)`
  Generate one block of numSamples samples (ndim * num_samples), populating design_matrix.

Private Member Functions

- `void compute_main_effects ()`
  builds a DDaceMainEffects::OneWayANOVA if mainEffectsFlag is set
- `boost::shared_ptr< DDaceSamplerBase > create_sampler (Model &model)`
  create a DDACE sampler
- `void resolve_samples_symbols ()`
  convenience function for resolving number of samples and number of symbols from input.
Private Attributes

- `unsigned short daceMethod`
  - `oas`, `lhs`, `oa_lhs`, `random`, `box_behnken`, `central_composite`, or `grid`
- `int samplesSpec`
  - initial specification of number of samples
- `int symbolsSpec`
  - initial specification of number of symbols
- `int numSamples`
  - current number of samples to be evaluated
- `int numSymbols`
  - current number of symbols to be used in generating the sample set (inversely related to number of replications)
- `const int seedSpec`
  - the user seed specification for the random number generator (allows repeatable results)
- `int randomSeed`
  - current seed for the random number generator
- `bool allDataFlag`
  - flag which triggers the update of allVars/allResponses for use by `Iterator::all_variables()` and `Iterator::all_responses()`
- `size_t numDACERuns`
  - counter for number of executions for this object
- `bool varyPattern`
  - flag for continuing the random number sequence from a previous execution (e.g., for surrogate-based optimization) so that multiple executions are repeatable but not correlated.
- `bool mainEffectsFlag`
  - flag which specifies main effects
- `std::vector<std::vector<int>> symbolMapping`
  - mapping of symbols for main effects calculations

Additional Inherited Members

13.40.1 Detailed Description

Wrapper class for the DDACE design of experiments library.

The `DDACEDesignCompExp` class provides a wrapper for DDACE, a C++ design of experiments library from the Computational Sciences and Mathematics Research (CSMR) department at Sandia’s Livermore CA site. This class uses design and analysis of computer experiments (DACE) methods to sample the design space spanned by the bounds of a `Model`. It returns all generated samples and their corresponding responses as well as the best sample found.

13.40.2 Constructor & Destructor Documentation

`DDACEDesignCompExp ( ProblemDescDB & problem_db, Model & model )`

primary constructor for building a standard DACE iterator

This constructor is called for a standard iterator built with data from `probDescDB`. References Dakota::abort_handler(), `DDACEDesignCompExp::daceMethod`, `DDACEDesignCompExp::mainEffectsFlag`, `Iterator::maxEvalConcurrency`, `Analyzer::numContinuousVars`, `Analyzer::numDiscreteIntVars`, `Analyzer::numDiscreteRealVars`, `Analyzer::numDiscreteStringVars`, and `DDACEDesignCompExp::numSamples`. 

13.40. DDACEDesignCompExp Class Reference

`DDACEDesignCompExp ( Model & model, int samples, int symbols, int seed, unsigned short sampling_method )`

Alternate constructor used for building approximations

This alternate constructor is used for instantiations on-the-fly, using only the incoming data. No problem description database queries are used.

References Dakota::abort_handler(), Iterator::maxEvalConcurrency, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, DDACEDesignCompExp::numSamples, and DDACEDesignCompExp::resolve_samples_symbols().

13.40.3 Member Function Documentation

```c++
void pre_run ( ) [protected], [virtual]
```

Pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

Pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s `pre_run()`, if implemented, typically before performing its own implementation steps.

Reimplemented from Analyzer.

References DDACEDesignCompExp::get_parameter_sets(), Analyzer::get_vbd_parameter_sets(), Iterator::iterated_Model, DDACEDesignCompExp::numSamples, Analyzer::pre_run(), DDACEDesignCompExp::resolve_samples_symbols(), and PStudyDACE::varBasedDecompFlag.

```c++
void core_run ( ) [protected], [virtual]
```

Core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References DDACEDesignCompExp::allDataFlag, Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, DDACEDesignCompExp::mainEffectsFlag, Analyzer::numLSqTerms, Analyzer::numObjFns, and Iterator::subIteratorFlag.

```c++
void post_run ( std::ostream & s ) [protected], [virtual]
```

Post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s `post_run()`, typically after performing its own implementation steps.

Reimplemented from Analyzer.

References Dakota::abort_handler(), Analyzer::allResponses, Analyzer::allSamples, SensAnalysisGlobal::compute_correlations(), DDACEDesignCompExp::compute_main_effects(), Analyzer::compute_vbd_stats(), DDACEDesignCompExp::create_sampler(), Iterator::iteratedModel, DDACEDesignCompExp::mainEffectsFlag, DDACEDesignCompExp::numSamples, Analyzer::post_run(), PStudyDACE::pStudyDACEsensGlobal, DDACEDesignCompExp::seedSpec, Iterator::subIteratorFlag, DDACEDesignCompExp::symbolMapping, and PStudyDACE::varBasedDecompFlag.
int num_samples() const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.
References DDACEDesignCompExp::numSamples.
Referenced by DDACEDesignCompExp::get_parameter_sets().

void resolve_samples_symbols() [private]

convenience function for resolving number of samples and number of symbols from input.

This function must define a combination of samples and symbols that is acceptable for a particular sampling algorithm. Users provide requests for these quantities, but this function must enforce any restrictions imposed by the sampling algorithms.

References Dakota::abort_handler(), DDACEDesignCompExp::daceMethod, Analyzer::numContinuousVars, DDACEDesignCompExp::numSamples, DDACEDesignCompExp::numSymbols, and Iterator::submethod_enum_to_string().

Referenced by DDACEDesignCompExp::DDACEDesignCompExp(), DDACEDesignCompExp::post_input(), and DDACEDesignCompExp::pre_run().

The documentation for this class was generated from the following files:

- DDACEDesignCompExp.hpp
- DDACEDesignCompExp.cpp

13.41 DirectApplicInterface Class Reference

Derived application interface class which spawns simulation codes and testers using direct procedure calls.

Inheritance diagram for DirectApplicInterface:

```
  Interface
  ApplicationInterface
  DirectApplicInterface
```

Public Member Functions

- **DirectApplicInterface** (const ProblemDescDB &problem_db)
  
  constructor

- **~DirectApplicInterface** ()
  
  destructor

- **void derived_map** (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)
  
  Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.

- **void derived_map_asynch** (const ParamResponsePair &pair)
  
  Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.

- **void wait_local_evaluations** (PRPQueue &prp_queue)
For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.

- void test_local_evaluations (PRPQueue &prp_queue)

For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version is nonblocking and will return without any completions if none are immediately available.

- int synchronous_local_analysis (int analysis_id)
- const StringArray & analysis_drivers () const

retrieve the analysis drivers specification for application interfaces

- void init_communicators_checks (int max_eval_concurrency)
- void set_communicators_checks (int max_eval_concurrency)

Protected Member Functions

- virtual int derived_map_if (const Dakota::String &if_name)

execute the input filter portion of a direct evaluation invocation

- virtual int derived_map_ac (const Dakota::String &ac_name)

execute an analysis code portion of a direct evaluation invocation

- virtual int derived_map_of (const Dakota::String &of_name)

execute the output filter portion of a direct evaluation invocation

- virtual void set_local_data (const Variables &vars, const ActiveSet &set)

convenience function for local test simulators which sets per-evaluation variable and active set attributes; derived classes reimplementing this likely need to invoke the base class API

- virtual void set_local_data (const Response &response)

convenience function for local test simulators which sets per-evaluation response attributes; derived classes reimplementing this likely need to invoke the base class API

- virtual void set_local_data (const Variables &vars, const ActiveSet &set, const Response &response)

convenience function for local test simulators which sets per-evaluation variable, active set, and response attributes; derived classes reimplementing this likely need to invoke the base class API

- void overlay_response (Response &response)

convenience function for local test simulators which overlays response contributions from multiple analyses using MPI_Reduce

Protected Attributes

- String iFilterName

name of the direct function input filter

- String oFilterName

name of the direct function output filter

- driver_t iFilterType

enum type of the direct function input filter

- driver_t oFilterType

enum type of the direct function output filter

- bool gradFlag

signals use of fnGrads in direct simulator functions

- bool hessFlag
signals use of fnHessians in direct simulator functions

- \texttt{size_t numFns}
  - number of functions in \texttt{fnVals}
- \texttt{size_t numVars}
  - total number of continuous and discrete variables
- \texttt{size_t numACV}
  - total number of continuous variables
- \texttt{size_t numADIV}
  - total number of discrete integer variables
- \texttt{size_t numADRV}
  - total number of discrete real variables
- \texttt{size_t numADSV}
  - total number of discrete string variables
- \texttt{size_t numDerivVars}
  - number of active derivative variables
- \texttt{unsigned short localDataView}
  - bit-wise record of which local data views are active; see enum \texttt{localData\_t}
- \texttt{RealVector xC}
  - continuous variables used within direct simulator fns
- \texttt{IntVector xDI}
  - discrete int variables used within direct simulator fns
- \texttt{RealVector xDR}
  - discrete real variables used within direct simulator fns
- \texttt{StringMultiArray xDS}
  - discrete string variables used within direct simulator fns
- \texttt{StringMultiArray xCLabels}
  - continuous variable labels
- \texttt{StringMultiArray xDILabels}
  - discrete integer variable labels
- \texttt{StringMultiArray xDRLabels}
  - discrete real variable labels
- \texttt{StringMultiArray xDSLabels}
  - discrete string variable labels
- \texttt{std::map< String, var\_t > varTypeMap}
  - map from variable label to enum
- \texttt{std::map< String, driver\_t > driverTypeMap}
  - map from driver name to enum
- \texttt{std::map< var\_t, Real > xCM}
  - map from \texttt{var\_t} enum to continuous value
- \texttt{std::map< var\_t, int > xDIM}
  - map from \texttt{var\_t} enum to discrete int value
- \texttt{std::map< var\_t, Real > xDRM}
  - map from \texttt{var\_t} enum to discrete real value
DirectApplicInterface Class Reference

- `std::map<var_t, String>` xDSM
  - Map from var_t enum to discrete string value
- `std::vector<var_t>` varTypeDVV
  - var_t enumerations corresponding to DVV components
- `std::vector<var_t>` xCMLabels
  - var_t enumerations corresponding to continuous variable labels
- `std::vector<var_t>` xDIMLabels
  - var_t enumerations corresponding to discrete integer variable labels
- `std::vector<var_t>` xDRMLabels
  - var_t enumerations corresponding to discrete real variable labels
- `std::vector<var_t>` xDSMLabels
  - var_t enumerations corresponding to discrete string variable labels
- `ShortArray` directFnASV
  - Class scope active set vector
- `SizetArray` directFnDVV
  - Class scope derivative variables vector
- `RealVector` fnVals
  - Response fn values within direct simulator fns
- `RealMatrix` fnGrads
  - Response fn gradients w/i direct simulator fns
- `RealSymMatrixArray` fnHessians
  - Response fn Hessians within direct fns
- `StringArray` analysisDrivers
  - The set of analyses within each function evaluation (from the analysis_drivers interface specification)
- `std::vector<driver_t>` analysisDriverTypes
  - Conversion of analysisDrivers to driver_t
- `size_t` analysisDriverIndex
  - The index of the active analysis driver within analysisDrivers
- `String2DArray` analysisComponents
  - The set of optional analysis components used by the analysis drivers (from the analysis_components interface specification)

Private Member Functions

- `void map_labels_to_enum` (StringMultiArrayConstView &src, std::vector<var_t> &dest)
  - Map labels in src to var_t in dest

13.41.1 Detailed Description

Derived application interface class which spawns simulation codes and testers using direct procedure calls. DirectApplicInterface uses a few linkable simulation codes and several internal member functions to perform parameter to response mappings.
13.41.2 Member Function Documentation

**int synchronous_local_analysis ( int analysis_id ) [inline], [virtual]**

This code provides the derived function used by `ApplicationInterface::serve_analyses_synch()`.
Reimplemented from `ApplicationInterface`.
References `DirectApplicInterface::analysisDriverIndex`, `DirectApplicInterface::analysisDrivers`, and `DirectApplicInterface::derived_map_ac()`.

**void init_communicators_checks ( int max_eval_concurrency ) [inline], [virtual]**

Process init issues as warnings since some contexts (e.g., `HierarchSurrModel`) initialize more configurations than will be used and `DirectApplicInterface` allows override by derived plug-ins.
Reimplemented from `ApplicationInterface`.
References `ApplicationInterface::check_asynchronous()`, and `ApplicationInterface::check_multiprocessor_asynchronous()`.

**void set_communicators_checks ( int max_eval_concurrency ) [inline], [virtual]**

Process run-time issues as hard errors.
Reimplemented from `ApplicationInterface`.
Reimplemented in `SerialDirectApplicInterface`, and `ParallelDirectApplicInterface`.
References Dakota::abort_handler(), `ApplicationInterface::check_asynchronous()`, and `ApplicationInterface::check_multiprocessor_asynchronous()`.

**int derived_map_ac ( const Dakota::String & ac_name ) [protected], [virtual]**

execute an analysis code portion of a direct evaluation invocation
When a direct analysis/filter is a member function, the (vars,set,response) data does not need to be passed through the API. If, however, non-member analysis/filter functions are added, then pass (vars,set,response) through to the non-member fns:

```cpp
// API declaration
int sim(const Variables& vars, const ActiveSet& set, Response& response);
// use of API within derived_map_ac()
if (ac_name == "sim")
   fail_code = sim(directFnVars, directFnActSet, directFnResponse);
```

Reimplemented in `SerialDirectApplicInterface`, `ParallelDirectApplicInterface`, `MatlabInterface`, `PythonInterface`, `TestDriverInterface`, and `ScilabInterface`.
References Dakota::abort_handler(), and `ApplicationInterface::analysisServerId`.
References by `DirectApplicInterface::derived_map()`, and `DirectApplicInterface::synchronous_local_analysis()`.
The documentation for this class was generated from the following files:

- `DirectApplicInterface.hpp`
- `DirectApplicInterface.cpp`

13.42 DiscrepancyCorrection Class Reference

Base class for discrepancy corrections.
Public Member Functions

- **DiscrepancyCorrection ()**
  - default constructor
- **DiscrepancyCorrection (Model &surr_model, const IntSet &surr_fn_indices, short corr_type, short corr_order)**
  - standard constructor
- **DiscrepancyCorrection (const IntSet &surr_fn_indices, size_t num_fns, size_t num_vars, short corr_type, short corr_order)**
  - alternate constructor
- **~DiscrepancyCorrection ()**
  - destructor
- **void initialize (Model &surr_model, const IntSet &surr_fn_indices, short corr_type, short corr_order)**
  - initialize the DiscrepancyCorrection data
- **void initialize (const IntSet &surr_fn_indices, size_t num_fns, size_t num_vars, short corr_type, short corr_order)**
  - initialize the DiscrepancyCorrection data
- **void initialize (const IntSet &surr_fn_indices, size_t num_fns, size_t num_vars, short corr_type, short corr_order, const String &approx_type)**
  - initialize the DiscrepancyCorrection data
- **void compute (const Variables &vars, const Response &truth_response, const Response &approx_response, bool quiet_flag=false)**
  - compute the correction required to bring approx_response into agreement with truth_response and store in {add,mult} Corrections
- **void compute (const Response &truth_response, const Response &approx_response, Response &discrepancy_response, bool quiet_flag=false)**
  - compute the correction required to bring approx_response into agreement with truth_response and store in discrepancy_response
- **void compute (const VariablesArray &vars_array, const ResponseArray &truth_response_array, const ResponseArray &approx_response, bool quiet_flag=false)**
  - compute the correction required to bring approx_response into agreement with truth_response as a function of the variables and store in {add,mult} Corrections
- **void apply (const Variables &vars, Response &approx_response, bool quiet_flag=false)**
  - apply the correction computed in compute() to approx_response
- **void compute_variance (const VariablesArray &vars_array, RealMatrix &approx_variance, bool quiet_flag=false)**
  - compute the variance of approx_response
- **short correction_type () const**
  - return correctionType
- **short correction_order () const**
  - return correctionOrder
- **short data_order () const**
  - return dataOrder
- **bool computed () const**
  - return correctionComputed
- **bool initialized () const**
  - return initializedFlag
Protected Attributes

- `IntSet surrogateFnIndices` for mixed response sets, this array specifies the response function subset that is approximated
- `bool initializedFlag` indicates that discrepancy correction instance has been initialized following construction
- `short correctionType` approximation correction approach to be used: `NO_CORRECTION`, `ADDITIONAL_CORRECTION`, `MULTIPLICATIVE_CORRECTION`, or `COMBINED_CORRECTION`.
- `short correctionOrder` approximation correction order to be used: 0, 1, or 2
- `short dataOrder` order of correction data in 3-bit format: overlay of 1 (value), 2 (gradient), and 4 (Hessian)
- `bool correctionComputed` flag indicating whether or not a correction has been computed and is available for application
- `size_t numFns` total number of response functions (of which surrogateFnIndices may define a subset)
- `size_t numVars` number of continuous variables active in the correction

Private Member Functions

- `void initialize_corrections ()` internal convenience function shared by overloaded `initialize()` variants
- `bool check_scaling (const RealVector &truth_fns, const RealVector &approx_fns)` define badScalingFlag
- `void compute_additive (const Response &truth_response, const Response &approx_response, int index, Real &discrep_fn, RealVector &discrep_grad, RealSymMatrix &discrep_hess)` internal convenience function for computing additive corrections between truth and approximate responses
- `void compute_multiplicative (const Response &truth_response, const Response &approx_response, int index, Real &discrep_fn, RealVector &discrep_grad, RealSymMatrix &discrep_hess)` internal convenience function for computing multiplicative corrections between truth and approximate responses
- `void apply_additive (const Variables &vars, Response &approx_response)` internal convenience function for applying additive corrections to an approximate response
- `void apply_multiplicative (const Variables &vars, Response &approx_response)` internal convenience function for applying multiplicative corrections to an approximate response
- `void apply_additive (const Variables &vars, RealVector &approx_fns)` internal convenience function for applying additive corrections to a set of response functions
- `void apply_multiplicative (const Variables &vars, RealVector &approx_fns)` internal convenience function for applying multiplicative corrections to a set of response functions
- `const Response & search_db (const Variables &search_vars, const ShortArray &search_asv)` search data pairs for missing approximation data
Private Attributes

- bool badScalingFlag
  flag used to indicate function values near zero for multiplicative corrections; triggers an automatic switch to additive corrections
- bool computeAdditive
  flag indicating the need for additive correction calculations
- bool computeMultiplicative
  flag indicating the need for multiplicative correction calculations
- String approxType
  string indicating the discrepancy approximation type
- SharedApproxData sharedData
  data that is shared among all correction Approximations
- std::vector< Approximation > addCorrections
  array of additive corrections; surrogate models of a model discrepancy function (formed from model differences)
- std::vector< Approximation > multCorrections
  array of multiplicative corrections; surrogate models of a model discrepancy function (formed from model ratios)
- Model surrModel
  shallow copy of the surrogate model instance as returned by Model::surrogate_model() (the DataFitSurrModel or HierarchSurrModel::lowFidelityModel instance)
- RealVector combineFactors
  factors for combining additive and multiplicative corrections. Each factor is the weighting applied to the additive correction and 1.-factor is the weighting applied to the multiplicative correction. The factor value is determined by an additional requirement to match the high fidelity function value at the previous correction point (e.g., previous trust region center). This results in a multipoint correction instead of a strictly local correction.
- Variables correctionPrevCenterPt
  copy of center point from the previous correction cycle
- RealVector truthFnsCenter
  truth function values at the current correction point
- RealVector approxFnsCenter
  Surrogate function values at the current correction point.
- RealMatrix approxGradsCenter
  Surrogate gradient values at the current correction point.
- RealVector truthFnsPrevCenter
  copy of truth function values at center of previous correction cycle
- RealVector approxFnsPrevCenter
  copy of approximate function values at center of previous correction cycle

13.42.1 Detailed Description

Base class for discrepancy corrections.

The DiscrepancyCorrection class provides common functions for computing and applying corrections to approximations.
13.42.2 Member Function Documentation

```cpp
void compute ( const Variables & vars, const Response & truth_response, const Response & approx_response, bool quiet_flag = false )
```

compute the correction required to bring approx_response into agreement with truth_response and store in \{add,mult\}Corrections

Compute an additive or multiplicative correction that corrects the approx_response to have 0th-order consistency (matches values), 1st-order consistency (matches values and gradients), or 2nd-order consistency (matches values, gradients, and Hessians) with the truth_response at a single point (e.g., the center of a trust region). The 0th-order, 1st-order, and 2nd-order corrections use scalar values, linear scaling functions, and quadratic scaling functions, respectively, for each response function.

References Response::active_set(), DiscrepancyCorrection::addCorrections, DiscrepancyCorrection::apply(), DiscrepancyCorrection::apply_additive(), DiscrepancyCorrection::apply_multiplicative(), DiscrepancyCorrection::approxFnsCenter, DiscrepancyCorrection::approxFnsPrevCenter, DiscrepancyCorrection::approxGradsCenter, DiscrepancyCorrection::approxType, DiscrepancyCorrection::badScalingFlag, DiscrepancyCorrection::check_scaling(), DiscrepancyCorrection::combineFactors, DiscrepancyCorrection::compute_additive(), DiscrepancyCorrection::compute_multiplicative(), DiscrepancyCorrection::computeAdditive, DiscrepancyCorrection::computeMultiplicative, Variables::continuous_variables(), Response::copy(), DiscrepancyCorrection::correctionComputed, DiscrepancyCorrection::correctionOrder, DiscrepancyCorrection::correctionPrevCenterPt, DiscrepancyCorrection::correctionType, DiscrepancyCorrection::dataOrder, Variables::discrete_int_variables(), Variables::discrete_real_variables(), Response::function_gradients(), Response::function_values(), Model::is_null(), DiscrepancyCorrection::multCorrections, DiscrepancyCorrection::numFns, DiscrepancyCorrection::numVars, ActiveSet::request_values(), DiscrepancyCorrection::sharedData, DiscrepancyCorrection::surrModel, DiscrepancyCorrection::surrogateFnIndices, DiscrepancyCorrection::truthFnsCenter, and DiscrepancyCorrection::truthFnsPrevCenter.

Referenced by HierarchSurrBasedLocalMinimizer::build(), NonDBayesCalibration::build_model_discrepancy(), DiscrepancyCorrection::compute(), DataFitSurrModel::derived_evaluate(), DataFitSurrModel::derived_synchronize(), and DataFitSurrModel::derived_synchronize_nowait().

The documentation for this class was generated from the following files:

- DiscrepancyCorrection.hpp
- DiscrepancyCorrection.cpp

13.43 DOTOptimizer Class Reference

Wrapper class for the DOT optimization library.

Inheritance diagram for DOTOptimizer:
Public Member Functions

- **DOTOptimizer** (ProblemDescDB &problem_db, Model &model)
  - standard constructor
- **DOTOptimizer** (const String &method_string, Model &model)
  - alternate constructor; construct without ProblemDescDB
- ~DOTOptimizer ()
  - destructor
- void **core_run ()**
  - core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Protected Member Functions

- void **initialize_run ()**
  - performs run-time set up

Private Member Functions

- void **initialize ()**
  - Shared constructor code.
- void **allocate_workspace ()**
  - Allocates workspace for the optimizer.
- void **allocate_constraints ()**
  - Allocates constraint mappings.

Private Attributes

- int **dotInfo**
  - INFO from DOT manual.
- int **dotFDSinfo**
  - internal DOT parameter NGOTOZ
- int **dotMethod**
  - METHOD from DOT manual.
- int **printControl**
  - IPRINT from DOT manual (controls output verbosity)
- RealArray **realCntlParmArray**
  - RPRM from DOT manual.
- IntArray **intCntlParmArray**
  - IPRM from DOT manual.
- RealVector **designVars**
  - array of design variable values passed to DOT
- Real **objFnValue**
  - value of the objective function passed to DOT
- RealVector **constraintValues**
  - array of nonlinear constraint values passed to DOT
• int realWorkSpaceSize
  size of realWorkSpace
• int intWorkSpaceSize
  size of intWorkSpace
• RealArray realWorkSpace
  real work space for DOT
• IntArray intWorkSpace
  int work space for DOT
• int numDotNlnConstr
  total number of nonlinear constraints seen by DOT
• int numDotLinConstr
  total number of linear constraints seen by DOT
• int numDotConstr
  total number of linear and nonlinear constraints seen by DOT
• SizetArray constraintMappingIndices
  a container of indices for referencing the corresponding Response constraints used in computing the DOT con-
  straints.
• RealArray constraintMappingMultipliers
  a container of multipliers for mapping the Response constraints to the DOT constraints.
• RealArray constraintMappingOffsets
  a container of offsets for mapping the Response constraints to the DOT constraints.

Additional Inherited Members

13.43.1 Detailed Description

Wrapper class for the DOT optimization library.

The DOTOptimizer class provides a wrapper for DOT, a commercial Fortran 77 optimization library from Vanderplaats Research and Development. It uses a reverse communication mode, which avoids the static member function issues that arise with function pointer designs (see NPSOLOptimizer and SNLLOptimizer).

The user input mappings are as follows: max_iterations is mapped into DOT's ITMAX parameter within its IPRM array, max_function_evaluations is implemented directly in the core_run() loop since there is no DOT parameter equivalent, convergence_tolerance is mapped into DOT's DELOBJ parameter (the relative convergence tolerance) within its RPRM array, output verbosity is mapped into DOT's IPRINT parameter within its function call parameter list (verbose: IPRINT = 7; quiet: IPRINT = 3), and optimization_type is mapped into DOT's MINMAX parameter within its function call parameter list. Refer to [Vanderplaats Research and Development, 1995] for information on IPRM, RPRM, and the DOT function call parameter list.

13.43.2 Member Function Documentation

void core_run( ) [virtual]
core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
Reimplemented from Iterator.
References Iterator::activeSet, Iterator::bestResponseArray, DOTOptimizer::constraintMappingIndices, DOTOptimizer::constraintMappingMultipliers, DOTOptimizer::constraintMappingOffsets, DOTOptimizer::constraintValues, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Model::current_response(), DOTOptimizer::designVars, DOTOptimizer::dotFDSinfo, DOTOptimizer::dotInfo, DOTOptimizer::dotMethod, Model::evaluate(), Response::function_gradients(), Response::function_values(), Model::gradient_type(), DOTOptimizer::intCntlParmArray, DOTOptimizer::intWorkSpace, DOTOptimizer::intWorkSpaceSize, Iterator::iteratedModel, Model::linear_eq_constraint_coeffs(), Model::linear_ineq_constraint_coeffs(), Optimizer::localObjectiveRecast, Iterator::maxFunctionEvals, Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), Minimizer::numContinuousVars, DOTOptimizer::numDotConstr, DOTOptimizer::numDotNlnConstr, Minimizer::numFunctions, Optimizer::numObjectiveFns, DOTOptimizer::objFnValue, Iterator::outputLevel, Model::primary_response_fn_sense(), DOTOptimizer::printControl, DOTOptimizer::realCntlParmArray, DOTOptimizer::realWorkSpace, DOTOptimizer::realWorkSpaceSize, ActiveSet::request_value(), ActiveSet::request_values(), Minimizer::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

### 13.43.3 Member Data Documentation

**int dotInfo** [private]

INFO from DOT manual.
- Information requested by DOT: 0=optimization complete, 1=get values, 2=get gradients
- Referenced by DOTOptimizer::core_run(), and DOTOptimizer::initialize_run().

**int dotFDSinfo** [private]

internal DOT parameter NGOTOZ
- the DOT parameter list has been modified to pass NGOTOZ, which signals whether DOT is finite-differencing (nonzero value) or performing the line search (zero value).
- Referenced by DOTOptimizer::core_run().

**int dotMethod** [private]

METHOD from DOT manual.
- For nonlinear constraints: 0/1 = dot_mmfd, 2 = dot_slp, 3 = dot_sqp. For unconstrained: 0/1 = dot_bfgs, 2 = dot_frcg.
- Referenced by DOTOptimizer::allocate_constraints(), DOTOptimizer::allocate_workspace(), and DOTOptimizer::core_run().

**int printControl** [private]

IPRINT from DOT manual (controls output verbosity)
- Values range from 0 (least output) to 7 (most output).
- Referenced by DOTOptimizer::core_run(), and DOTOptimizer::DOTOptimizer().

**RealArray realCntlParmArray** [private]

RPRM from DOT manual.
- Array of real control parameters.
- Referenced by DOTOptimizer::core_run(), and DOTOptimizer::initialize().
**IntArray intCntlParmArray**  [private]

IPRM from DOT manual.

Array of integer control parameters.

Referenced by DOTOptimizer::core_run(), and DOTOptimizer::initialize().

**RealVector constraintValues**  [private]

array of nonlinear constraint values passed to DOT

This array must be of nonzero length and must contain only one-sided inequality constraints which are \( \leq 0 \)
(which requires a transformation from 2-sided inequalities and equalities).

Referenced by DOTOptimizer::allocate_constraints(), and DOTOptimizer::core_run().

**SizetArray constraintMappingIndices**  [private]

a container of indices for referencing the corresponding Response constraints used in computing the DOT constraints.

The length of the container corresponds to the number of DOT constraints, and each entry in the container points to the corresponding DAKOTA constraint.

Referenced by DOTOptimizer::allocate_constraints(), and DOTOptimizer::core_run().

**RealArray constraintMappingMultipliers**  [private]

a container of multipliers for mapping the Response constraints to the DOT constraints.

The length of the container corresponds to the number of DOT constraints, and each entry in the container stores a multiplier for the DAKOTA constraint identified with constraintMappingIndices. These multipliers are currently +1 or -1.

Referenced by DOTOptimizer::allocate_constraints(), and DOTOptimizer::core_run().

**RealArray constraintMappingOffsets**  [private]

a container of offsets for mapping the Response constraints to the DOT constraints.

The length of the container corresponds to the number of DOT constraints, and each entry in the container stores an offset for the DAKOTA constraint identified with constraintMappingIndices. These offsets involve inequality bounds or equality targets, since DOT assumes constraint allowables = 0.

Referenced by DOTOptimizer::allocate_constraints(), and DOTOptimizer::core_run().

The documentation for this class was generated from the following files:

- DOTOptimizer.hpp
- DOTOptimizer.cpp

---

**13.44 JEGAOptimizer::Driver Class Reference**

A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.

Inherits Driver.
Public Member Functions

- GeneticAlgorithm * ExtractAllData (const AlgorithmConfig &algConfig)
  
  Reads all required data from the problem description database stored in the supplied algorithm config.

- DesignOFSortSet PerformIterations (GeneticAlgorithm *theGA)
  
  Performs the required iterations on the supplied GA.

- void DestroyAlgorithm (GeneticAlgorithm *theGA)
  
  Deletes the supplied GA.

- Driver (const ProblemConfig &probConfig)
  
  Default constructs a Driver.

13.44.1 Detailed Description

A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.

This is necessary because DAKOTA requires that all problem information be extracted from the problem description DB at the time of Optimizer construction and the front end does it all in the execute algorithm method which must be called in core_run.

13.44.2 Constructor & Destructor Documentation

Driver ( const ProblemConfig & probConfig ) [inline]

Default constructs a Driver.

Parameters

| probConfig | The definition of the problem to be solved by this Driver whenever ExecuteAlgorithm is called. |

The problem can be solved in multiple ways by multiple algorithms even using multiple different evaluators by issuing multiple calls to ExecuteAlgorithm with different AlgorithmConfigs.

13.44.3 Member Function Documentation

GeneticAlgorithm* ExtractAllData ( const AlgorithmConfig & algConfig ) [inline]

Reads all required data from the problem description database stored in the supplied algorithm config.

The returned GA is fully configured and ready to be run. It must also be destroyed at some later time. You MUST call DestroyAlgorithm for this purpose. Failure to do so could result in a memory leak and an eventual segmentation fault! Be sure to call DestroyAlgorithm prior to destroying the algorithm config that was used to create it!

This is just here to expose the base class method to users.

Parameters

| algConfig | The fully loaded configuration object containing the database of parameters for the algorithm to be run on the known problem. |

Returns

The fully configured and loaded GA ready to be run using the PerformIterations method.

Referenced by JEGAOptimizer::core_run().
DesignOFSortSet PerformIterations ( GeneticAlgorithm * theGA ) [inline]

Performs the required iterations on the supplied GA.
This includes the calls to AlgorithmInitialize and AlgorithmFinalize and logs some information if appropriate.
This is just here to expose the base class method to users.

Parameters

| theGA | The GA on which to perform iterations. This parameter must be non-null. |

Returns

The final solutions reported by the supplied GA after all iterations and call to AlgorithmFinalize.

Referenced by JEGAOptimizer::core_run().

void DestroyAlgorithm ( GeneticAlgorithm * theGA ) [inline]

Deletes the supplied GA.
Use this method to destroy a GA after all iterations have been run. This method knows if the log associated with the GA was created here and needs to be destroyed as well or not.
This is just here to expose the base class method to users.
Be sure to use this prior to destroying the algorithm config object which contains the target. The GA destructor needs the target to be in tact.

Parameters

| theGA | The algorithm that is no longer needed and thus must be destroyed. |

Referenced by JEGAOptimizer::core_run().
The documentation for this class was generated from the following file:

- JEGAOptimizer.cpp

### 13.45 EffGlobalMinimizer Class Reference

Implementation of Efficient Global Optimization/Least Squares algorithms.

Inheritance diagram for EffGlobalMinimizer:

```
EffGlobalMinimizer
  └── SurrBasedMinimizer
    └── Minimizer
      └── Iterator
```

**Public Member Functions**

- EffGlobalMinimizer (ProblemDescDB &problem_db, Model &model)
13.45. **EFFGLOBALMINIMIZER CLASS REFERENCE**

`standard constructor`

- ~EffGlobalMinimizer ()
  
  alternate constructor for instantiations "on the fly"

- void core_run ()
  
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

- const Model & algorithm_space_model () const

**Private Member Functions**

- void minimize_surrogates_on_model ()
  
  called by minimize_surrogates for setUpType == "model"

- void get_best_sample ()
  
  called by minimize_surrogates for setUpType == "user functions"

- Real expected_improvement (const RealVector &means, const RealVector &variances)
  
  expected improvement function for the GP

- RealVector expected_violation (const RealVector &means, const RealVector &variances)
  
  expected violation function for the constraint functions

- void update_penalty ()
  
  initialize and update the penaltyParameter

**Static Private Member Functions**

- static void EIF_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  
  static function used as the objective function in the Expected Improvement (EIF) problem formulation for PMA

**Private Attributes**

- String setUpType
  
  controls iteration mode: "model" (normal usage) or "user functions" (user-supplied functions mode for "on the fly" instantiations).

- Model fHatModel
  
  GP model of response, one approximation per response function.

- Model eifModel
  
  recast model which assimilates mean and variance to solve the max(EIF) sub-problem

- Real meritFnStar
  
  minimum penalized response from among true function evaluations

- RealVector truthFnStar
  
  true function values corresponding to the minimum penalized response

- RealVector varStar
  
  point that corresponds to the optimal value meritFnStar

- short dataOrder
  
  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format; user may override responses spec
Static Private Attributes

- static EffGlobalMinimizer * effGlobalInstance
  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

13.45.1 Detailed Description

Implementation of Efficient Global Optimization/Least Squares algorithms.

The EffGlobalMinimizer class provides an implementation of the Efficient Global Optimization algorithm developed by Jones, Schonlau, & Welch as well as adaptation of the concept to nonlinear least squares.

13.45.2 Constructor & Destructor Documentation

~EffGlobalMinimizer ( )
alternate constructor for instantiations ”on the fly”
destructor

13.45.3 Member Function Documentation

void core_run ( ) [virtual]
core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
  Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
  Reimplemented from Iterator.
  References Dakota::abort_handler(), EffGlobalMinimizer::minimize_surrogates_on_model(), and EffGlobalMinimizer::setUpType.

const Model & algorithm_space_model ( ) const [inline], [virtual]
default definition that gets redefined in selected derived Minimizers
  Reimplemented from Minimizer.
  References EffGlobalMinimizer::fHatModel.

void get_best_sample ( ) [private]
called by minimize_surrogates for setUpType == ”user_functions”
  determine best solution from among sample data for expected improvoment function
  References Model::approximation_data(), SurrBasedMinimizer::augmented_lagrangian_merit(), Model::continuous_variables(), Dakota::copy_data(), Model::current_response(), Model::evaluate(), EffGlobalMinimizer::fHatModel, Response::function_values(), Iterator::iteratedModel, EffGlobalMinimizer::meritFnStar, Minimizer::numFunctions, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), EffGlobalMinimizer::truthFnStar, and EffGlobalMinimizer::varStar.
  Referenced by EffGlobalMinimizer::minimize_surrogates_on_model().
  The documentation for this class was generated from the following files:
  - EffGlobalMinimizer.hpp
  - EffGlobalMinimizer.cpp
13.46 EmbedHybridMetaIterator Class Reference

Meta-iterator for closely-coupled hybrid iteration, typically involving the embedding of local search methods within global search methods.

Inheritance diagram for EmbedHybridMetaIterator:

```
  EmbedHybridMetaIterator
     |_____________________
       |                   |
  MetaIterator
     |_____________________
       |                   |
  Iterator
```

Public Member Functions

- `EmbedHybridMetaIterator (ProblemDescDB &problem_db)`
  * standard constructor
- `EmbedHybridMetaIterator (ProblemDescDB &problem_db, Model &model)`
  * alternate constructor
- `~EmbedHybridMetaIterator ()`
  * destructor

Protected Member Functions

- `void core_run ()`
  * Performs the hybrid iteration by executing global and local iterators, using a set of models that may vary in fidelity.
- `void derived_init_communicators (ParLevLIter pl_iter)`
  * derived class contributions to initialing the communicators associated with this Iterator instance
- `void derived_set_communicators (ParLevLIter pl_iter)`
  * derived class contributions to setting the communicators associated with this Iterator instance
- `void derived_free_communicators (ParLevLIter pl_iter)`
  * derived class contributions to freeing the communicators associated with this Iterator instance
- `IntIntPair estimate_partition_bounds ()`
  * estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- `const Variables & variables_results () const`
  * return the final solution from the embedded hybrid (variables)
- `const Response & response_results () const`
  * return the final solution from the embedded hybrid (response)

Private Attributes

- `Iterator globalIterator`
  * the top-level outer iterator (e.g., global minimizer)
- `Model globalModel`
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the model employed by the top-level outer iterator

• Iterator localIterator

  the inner iterator (e.g., local minimizer)

• Model localModel

  the model employed by the inner iterator

• bool singlePassedModel

  use of constructor that enforces use of a single passed Model

• Real localSearchProb

  the probability of running a local search refinement within phases of the global minimization for tightly-coupled hybrids

Additional Inherited Members

13.46.1 Detailed Description

Meta-iterator for closely-coupled hybrid iteration, typically involving the embedding of local search methods within global search methods.

This meta-iterator uses multiple methods in close coordination, generally using a local search minimizer repeatedly within a global minimizer (the local search minimizer refines candidate minima which are fed back to the global minimizer).

The documentation for this class was generated from the following files:

• EmbedHybridMetaIterator.hpp
• EmbedHybridMetaIterator.cpp

13.47 Environment Class Reference

Base class for the environment class hierarchy.

Inheritance diagram for Environment:

```
Environment
     +-- ExecutableEnvironment
     +-- LibraryEnvironment
```

Public Member Functions

• Environment ()

  default constructor: empty envelope

• Environment (int argc, char *argv[])

  envelope constructor for ExecutableEnvironment letter

• Environment (ProgramOptions prog_opts)

• Environment (MPI_Comm dakota_mpi_comm, ProgramOptions prog_opts=ProgramOptions())

• Environment (const String &env_type)

  envelope constructor for letter type identified by String
• **Environment** (const Environment &env)
  
  *copy constructor*

• virtual ~Environment ()

  *destructor*

• **Environment** operator= (const Environment &env)

  *assignment operator*

• virtual void execute ()

  *the run function for the environment: invoke the iterator(s) on the model(s). Called from main.cpp.*

• bool check () const

  *Print status of check and return true if in a "check" mode, including version and help. Return false if proceeding to a run mode.*

• MPIManager & mpi_manager ()

  *return mpiManager*

• ProgramOptions & program_options ()

  *return programOptions*

• OutputManager & output_manager ()

  *return outputManager*

• ParallelLibrary & parallel_library ()

  *return parallelLib*

• ProblemDescDB & problem_description_db ()

  *return probDescDB*

• const Variables & variables_results () const

  *return the final environment solution (variables)*

• const Response & response_results () const

  *return the final environment solution (response)*

• void exit_mode (const String &mode="exit")

  *allow environment clients to set Dakota exit behavior (throw vs. exit)*

### Protected Member Functions

• Environment (BaseConstructor)

  *constructor initializes the base class part of default-constructed letters*

• Environment (BaseConstructor, int argc, char *argv[])

  *constructor initializes the base class part of executable letter classes*

• Environment (BaseConstructor, ProgramOptions prog_opts, MPI_Comm dakota_mpi_comm=MPI_COMM_WORLD)

  *constructor initializes the base class part of library letter classes*

• void parse (bool check_bcast_database=true, DbCallbackFunctionPtr callback=NULL, void *callback_data=NULL)

  *parse inputs, callbacks, and optionally check and broadcast*

• void construct ()

  *Instantiate topLevelIterator;*

• void destruct ()

  *Dealocate parallel partitioning for topLevelIterator;*

• bool assign_model_pointer () const
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Protected Attributes

- MPIManager mpiManager
  the MPI manager instance
- ProgramOptions programOptions
  the command line options manager
- OutputManager outputManager
  (tagged) output stream manager
- ParallelLibrary parallelLib
  the parallel library instance
- ProblemDescDB probDescDB
  the parser database instance
- Iterator topLevelIterator
  the top level (meta-)iterator
- UsageTracker usageTracker
  tool for Dakota usage tracking (this is a thin wrapper class)

Private Member Functions

- Environment * get_environment (const String &env_type)
  Used by the envelope to instantiate the correct letter class.

Private Attributes

- Environment * environmentRep
  pointer to the letter (initialized only for the envelope)
- int referenceCount
  number of objects sharing environmentRep

13.47.1 Detailed Description

Base class for the environment class hierarchy.

The Environment class is the base class for the class hierarchy providing the top level control in DAKOTA. The environment is responsible for creating and managing iterators and models. For memory efficiency and enhanced polymorphism, the environment hierarchy employs the ”letter/envelope idiom” (see Coplien ”Advanced C++”, p. 133), for which the base class (Environment) serves as the envelope and one of the derived classes (selected in Environment::get_environment()) serves as the letter.

13.47.2 Constructor & Destructor Documentation

Environment ( )
default constructor: empty envelope

Default envelope constructor. environmentRep is NULL in this case, which makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.
Environment ( int argc, char * argv[] )
envelope constructor for ExecutableEnvironment letter

Envelope constructor for ExecutableEnvironment. Selection of derived type by get_environment() is not necessary in this case.
References Dakota::abort_handler(), and Environment::environmentRep.

Environment ( ProgramOptions prog_opts )
Envelope constructor for LibraryEnvironment. Selection of derived type by get_environment() is not necessary in this case.
References Dakota::abort_handler(), and Environment::environmentRep.

Environment ( MPI_Comm dakota_mpi_comm, ProgramOptions prog_opts = ProgramOptions () )
Envelope constructor for LibraryEnvironment. Selection of derived type by get_environment() is not necessary in this case.
References Dakota::abort_handler(), and Environment::environmentRep.

Environment ( const String & env_type )
envelope constructor for letter type identified by String

Alternate construction by String. Envelope constructor invokes get_environment() which instantiates a derived class letter; the derived constructor selects a BaseConstructor constructor in its initialization list to avoid the recursion of a base class constructor calling get_environment() again.
References Dakota::abort_handler(), Environment::environmentRep, and Environment::get_environment().

Environment ( const Environment & env )
copy constructor
Copy constructor manages sharing of environmentRep and incrementing of referenceCount.
References Environment::environmentRep, and Environment::referenceCount.

~Environment( ) [virtual]
destructor
Destructor decrements referenceCount and only deletes environmentRep when referenceCount reaches zero.
References Environment::destruct(), Environment::environmentRep, and Environment::referenceCount.

Environment ( BaseConstructor ) [protected]
constructor initializes the base class part of default-constructed letters

This letter constructor initializes base class data for inherited environments that are default constructed. Since the letter IS the representation, its representation pointer is set to NULL (an uninitialized pointer causes problems in ~Environment).
Use cases: library with no options, no MPI comm
References ProgramOptions::exit_mode(), Environment::exit_mode(), WorkdirHelper::initialize(), and Environment::programOptions.
**Environment ( BaseConstructor, int argc, char * argv[] ) [protected]**

constructor initializes the base class part of executable letter classes

This letter constructor initializes base class data for inherited environments: instantiate/initialize the environment, options, parallel library, and problem description database objects. Since the letter IS the representation, its representation pointer is set to NULL (an uninitialized pointer causes problems in ∼Environment).

Use cases: executable with command-line args

References ProgramOptions::exit_mode(), Environment::exit_mode(), WorkdirHelper::initialize(), and Environment::programOptions.

**Environment ( BaseConstructor, ProgramOptions prog_opts, MPI_Comm dakota_mpi_comm = MPI_COMM_WORLD ) [protected]**

constructor initializes the base class part of library letter classes

This letter constructor initializes base class data for inherited environments. Since the letter IS the representation, its representation pointer is set to NULL (an uninitialized pointer causes problems in ∼Environment).

Use cases: library with program options library with program options and MPI comm

References ProgramOptions::exit_mode(), Environment::exit_mode(), WorkdirHelper::initialize(), and Environment::programOptions.

### 13.47.3 Member Function Documentation

**Environment operator= ( const Environment & env )**

assignment operator


References Environment::environmentRep, and Environment::referenceCount.

**void exit_mode ( const String & mode = "exit" )**

allow environment clients to set Dakota exit behavior (throw vs. exit)

Set the global variable controlling Dakota’s exit behavior. Call with no arguments to reset to default behavior.

References Dakota::abort_handler(), and Dakota::abort_mode.

Referenced by Environment::Environment(), and run_dakota_data().

**void parse ( bool check_bcast_database = true, DbCallbackFunctionPtr callback = NULL, void * callback_data = NULL ) [protected]**

parse inputs, callbacks, and optionally check and broadcast

Parse input file and invoked any callbacks, then optionally check and sync database if check_bcast_database = true.

References ProblemDescDB::check_and_broadcast(), ProgramOptions::input_file(), ProgramOptions::input_string(), ProblemDescDB::parse_inputs(), Environment::probDescDB, and Environment::programOptions.

Referenced by ExecutableEnvironment::ExecutableEnvironment(), and LibraryEnvironment::LibraryEnvironment().

**Environment * get_environment ( const String & env_type ) [private]**

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize environmentRep to the appropriate derived type, as given by the environmentName attribute.
Referenced by Environment::Environment().
The documentation for this class was generated from the following files:

- DakotaEnvironment.hpp
- DakotaEnvironment.cpp

### 13.48 NomadOptimizer::Evaluator Class Reference

NOMAD-based `Evaluator` class.
Inherits `Evaluator`.

#### Public Member Functions

- **Evaluator** (const NOMAD::Parameters &p, Model &model)
  
  Constructor.

- **~Evaluator** (void)
  
  Destructor.

- bool eval_x (NOMAD::Eval_Point &x, const NOMAD::Double &h_max, bool &count_eval) const
  
  Main Evaluation Method.

- void set_constraint_map (int numNomadNonlinearIneqConstraints, int numNomadNonlinearEqConstraints, 
  std::vector<int> constrMapIndices, std::vector<double> constrMapMultipliers, std::vector<double> constrMapOffsets)
  
  publishes constraint transformation

- void set_surrogate_usage (std::string useSurrogate)
  
  publishes surrogate usage

#### Private Attributes

- Model & _model
- int n_cont
- int n_disc_int
- int n_disc_real
- int numNomadNonlinearIneqConstr
  
  Number of nonlinear constraints after put into Nomad format.

- int numNomadNonlinearEqConstr
  
  std::vector<int> constrMapIndices
  
  map from Dakota constraint number to Nomad constraint number

- std::vector<double> constrMapMultipliers
  
  multipliers for constraint transformations

- std::vector<double> constrMapOffsets
  
  offsets for constraint transformations

- std::string useSgte
  
  defines use of surrogate in NOMAD
13.48.1 Detailed Description

NOMAD-based Evaluator class.

The NOMAD process requires an evaluation step, which calls the Simulation program. In the simplest version of this call, NOMAD executes the black box executable, which proceeds to write a file in a NOMAD-compatible format, which NOMAD reads to continue the process.

Because DAKOTA files are different form NOMAD files, and the simulations processed by DAKOTA already produce DAKOTA-compatible files, we cannot use this method for NOMAD. Instead, we implement the Nomad-Evaluator class, which takes the NOMAD inputs and passes them to DAKOTA's Interface for processing. The evaluator then passes the evaluation Responses into the NOMAD objects for further analysis.

13.48.2 Constructor & Destructor Documentation

Evaluator ( const NOMAD::Parameters & p, Model & model )

Constructor.

NOMAD Evaluator Constructor

Parameters

<table>
<thead>
<tr>
<th>p</th>
<th>NOMAD Parameters object</th>
</tr>
</thead>
<tbody>
<tr>
<td>model</td>
<td>DAKOTA Model object</td>
</tr>
</tbody>
</table>

13.48.3 Member Function Documentation

bool eval_x ( NOMAD::Eval_Point & x, const NOMAD::Double & h_max, bool & count_eval ) const

Main Evaluation Method.

Method that handles the communication between the NOMAD search process and the Black Box Evaluation managed by DAKOTA's Interface.

Parameters

<table>
<thead>
<tr>
<th>x</th>
<th>Object that contains the points that need to evaluated. Once the evaluation is completed, this object also stores the output back to be read by NOMAD.</th>
</tr>
</thead>
<tbody>
<tr>
<td>h_max</td>
<td>Current value of the barrier parameter. Not used in this implementation.</td>
</tr>
<tr>
<td>count_eval</td>
<td>Flag that indicates whether this evaluation counts towards the max number of evaluations, often set to false when the evaluation does not meet certain costs during expensive evaluations. Not used in this implementation.</td>
</tr>
</tbody>
</table>

Returns

ttrue if the evaluation was successful; false otherwise.

References Dakota::set_index_to_value().

The documentation for this class was generated from the following files:

- NomadOptimizer.hpp
- NomadOptimizer.cpp

13.49 JEGAOptimizer::Evaluator Class Reference

An evaluator specialization that knows how to interact with Dakota.

Inherits GeneticAlgorithmEvaluator.
Public Member Functions

- virtual bool Evaluate (DesignGroup &group)
  
  Does evaluation of each design in group.

- virtual bool Evaluate (Design &des)
  
  This method cannot be used!!

- virtual std::string GetName () const
  
  Returns the proper name of this operator.

- virtual std::string GetDescription () const
  
  Returns a full description of what this operator does and how.

- virtual GeneticAlgorithmOperator ∗ Clone (GeneticAlgorithm &algorithm) const
  
  Creates and returns a pointer to an exact duplicate of this operator.

- Evaluator (GeneticAlgorithm &algorithm, Model &model)
  
  Constructs a Evaluator for use by algorithm.

- Evaluator (const Evaluator &copy)
  
  Copy constructs a Evaluator.

- Evaluator (const Evaluator &copy, GeneticAlgorithm &algorithm, Model &model)
  
  Copy constructs a Evaluator for use by algorithm.

Static Public Member Functions

- static const std::string & Name ()
  
  Returns the proper name of this operator.

- static const std::string & Description ()
  
  Returns a full description of what this operator does and how.

Protected Member Functions

- void SeparateVariables (const Design &from, RealVector &intoCont, IntVector &intoDiscInt, RealVector &intoDiscReal, StringMultiArray &intoDiscString) const
  
  This method fills intoCont, intoDiscInt and intoDiscReal appropriately using the values of from.

- void RecordResponses (const RealVector &from, Design &into) const
  
  Records the computed objective and constraint function values into into.

- std::size_t GetNumberNonLinearConstraints () const
  
  Returns the number of non-linear constraints for the problem.

- std::size_t GetNumberLinearConstraints () const
  
  Returns the number of linear constraints for the problem.

Private Member Functions

- Evaluator (GeneticAlgorithm &algorithm)
  
  This constructor has no implementation and cannot be used.

Private Attributes

- Model & _model
  
  The Model known by this evaluator.
13.49.1 Detailed Description

An evaluator specialization that knows how to interact with Dakota.
This evaluator knows how to use the model to do evaluations both in synchronous and asynchronous modes.

13.49.2 Constructor & Destructor Documentation

Evaluator ( GeneticAlgorithm & algorithm, Model & model ) [inline]

Constructs a Evaluator for use by algorithm.
The optimizer is needed for purposes of variable scaling.

Parameters

<table>
<thead>
<tr>
<th>algorithm</th>
<th>The GA for which the new evaluator is to be used.</th>
</tr>
</thead>
<tbody>
<tr>
<td>model</td>
<td>The model through which evaluations will be done.</td>
</tr>
</tbody>
</table>

Evaluator ( const Evaluator & copy ) [inline]

Copy constructs a Evaluator.

Parameters

| copy | The evaluator from which properties are to be duplicated into this. |

Evaluator ( const Evaluator & copy, GeneticAlgorithm & algorithm, Model & model ) [inline]

Copy constructs a Evaluator for use by algorithm.
The optimizer is needed for purposes of variable scaling.

Parameters

<table>
<thead>
<tr>
<th>copy</th>
<th>The existing Evaluator from which to retrieve properties.</th>
</tr>
</thead>
<tbody>
<tr>
<td>algorithm</td>
<td>The GA for which the new evaluator is to be used.</td>
</tr>
<tr>
<td>model</td>
<td>The model through which evaluations will be done.</td>
</tr>
</tbody>
</table>

Evaluator ( GeneticAlgorithm & algorithm ) [private]

This constructor has no implementation and cannot be used.
This constructor can never be used. It is provided so that this operator can still be registered in an operator
registry even though it can never be instantiated from there.

Parameters

| algorithm | The GA for which the new evaluator is to be used. |

13.49.3 Member Function Documentation

static const std::string& Name ( ) [inline], [static]

Returns the proper name of this operator.

Returns

The string "DAKOTA JEGA Evaluator".
static const std::string& Description( ) [inline], [static]

Returns a full description of what this operator does and how.

The returned text is:

This evaluator uses Sandia’s DAKOTA optimization software to evaluate the passed in Designs. This makes it possible to take advantage of the fact that DAKOTA is designed to run on massively parallel machines.

Returns

A description of the operation of this operator.

void SeparateVariables( const Design& from, RealVector& intoCont, IntVector& intoDiscInt, RealVector& intoDiscReal, StringMultiArray& intoDiscString ) const [protected]

This method fills intoCont, intoDiscInt and intoDiscReal appropriately using the values of from.

The discrete integer design variable values are placed in intoDiscInt, the discrete real design variable values are placed in intoDiscReal, and the continuum are placed into intoCont. The values are written into the vectors from the beginning so any previous contents of the vectors will be overwritten.

Parameters

<table>
<thead>
<tr>
<th>from</th>
<th>The Design class object from which to extract the discrete design variable values.</th>
</tr>
</thead>
<tbody>
<tr>
<td>intoDiscInt</td>
<td>The vector into which to place the extracted discrete integer values.</td>
</tr>
<tr>
<td>intoDiscReal</td>
<td>The vector into which to place the extracted discrete real values.</td>
</tr>
<tr>
<td>intoCont</td>
<td>The vector into which to place the extracted continuous values.</td>
</tr>
</tbody>
</table>

References JEGAOptimizer::Evaluator::model, Model::cv(), Model::discrete_int_sets(), Model::discrete_string_values(), Model::div(), Model::drv(), Model::dsv(), and Dakota::set_index_to_value().

void RecordResponses( const RealVector& from, Design& into ) const [protected]

Records the computed objective and constraint function values into into.

This method takes the response values stored in from and properly transfers them into the into design.

The response vector from is expected to contain values for each objective function followed by values for each non-linear constraint in the order in which the info objects were loaded into the target by the optimizer class.

Parameters

<table>
<thead>
<tr>
<th>from</th>
<th>The vector of responses to install into into.</th>
</tr>
</thead>
<tbody>
<tr>
<td>into</td>
<td>The Design to which the responses belong and into which they must be written.</td>
</tr>
</tbody>
</table>

std::size_t GetNumberNonLinearConstraints( ) const [inline], [protected]

Returns the number of non-linear constraints for the problem.

This is computed by adding the number of non-linear equality constraints to the number of non-linear inequality constraints. These values are obtained from the model.

Returns

The total number of non-linear constraints.
std::size_t GetNumberOfLinearConstraints() const [inline], [protected]

Returns the number of linear constraints for the problem.

This is computed by adding the number of linear equality constraints to the number of linear inequality constraints. These values are obtained from the model.

Returns

The total number of linear constraints.

bool Evaluate(DesignGroup & group) [virtual]

Does evaluation of each design in group.

This method uses the Model known by this class to get Designs evaluated. It properly formats the Design class information in a way that Dakota will understand and then interprets the Dakota results and puts them back into the Design class object. It respects the asynchronous flag in the Model so evaluations may occur synchronously or asynchronously.

Prior to evaluating a Design, this class checks to see if it is marked as already evaluated. If it is, then the evaluation of that Design is not carried out. This is not strictly necessary because Dakota keeps track of evaluated designs and does not re-evaluate. An exception is the case of a population read in from a file complete with responses where Dakota is unaware of the evaluations.

Parameters

| group | The group of Design class objects to be evaluated. |

Returns

true if all evaluations completed and false otherwise.

virtual bool Evaluate(Design & des) [inline], [virtual]

This method cannot be used!!

This method does nothing and cannot be called. This is because in the case of asynchronous evaluation, this method would be unable to conform. It would require that each evaluation be done in a synchronous fashion.

Parameters

| des | A Design that would be evaluated if this method worked. |

Returns

Would return true if the Design were evaluated and false otherwise. Never actually returns here. Issues a fatal error. Otherwise, it would always return false.

virtual std::string GetName() const [inline], [virtual]

Returns the proper name of this operator.

Returns

See Name().
virtual std::string GetDescription () const [inline], [virtual]
Returns a full description of what this operator does and how.
Returns
    See Description().

virtual GeneticAlgorithmOperator* Clone ( GeneticAlgorithm & algorithm ) const [inline], [virtual]
Creates and returns a pointer to an exact duplicate of this operator.
Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>algorithm</td>
<td>The GA for which the clone is being created.</td>
</tr>
</tbody>
</table>

Returns
    A clone of this operator.

13.49.4 Member Data Documentation

Model& _model [private]
The Model known by this evaluator.
It is through this model that evaluations will take place.
Referenced by JEGAOptimizer::Evaluator::SeparateVariables().
The documentation for this class was generated from the following file:
- JEGAOptimizer.cpp

13.50 JEGAOptimizer::EvaluatorCreator Class Reference

A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.
Inherits EvaluatorCreator.

Public Member Functions
- virtual GeneticAlgorithmEvaluator* CreateEvaluator (GeneticAlgorithm &alg)
  Overriden to return a newly created Evaluator.
- EvaluatorCreator (Model &theModel)
  Constructs an EvaluatorCreator using the supplied model.

Private Attributes
- Model & _theModel
  The user defined model to be passed to the constructor of the Evaluator.

13.50.1 Detailed Description

A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.
13.50.2 Constructor & Destructor Documentation

EvaluatorCreator ( Model & theModel ) [inline]

Constructs an EvaluatorCreator using the supplied model.
13.50.3 Member Function Documentation

virtual GeneticAlgorithmEvaluator* CreateEvaluator ( GeneticAlgorithm & alg ) [inline], [virtual]

Overridden to return a newly created Evaluator.

The GA will assume ownership of the evaluator so we needn’t worry about keeping track of it for destruction. The additional parameters needed by the Evaluator are stored as members of this class at construction time.

Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>alg</td>
<td>The GA for which the evaluator is to be created.</td>
</tr>
</tbody>
</table>

Returns

A pointer to a newly created Evaluator.

The documentation for this class was generated from the following file:

- JEGAOptimizer.cpp

13.51 ExecutableEnvironment Class Reference

Environment corresponding to execution as a stand-alone application.

Inheritance diagram for ExecutableEnvironment:

```
Environment

ExecutableEnvironment
```

Public Member Functions

- `ExecutableEnvironment ()`
  
  default constructor

- `ExecutableEnvironment (int argc, char *argv[])`
  
  constructor

- `~ExecutableEnvironment ()`
  
  destructor

- `void execute ()`
  
  the run function for the environment: invoke the iterator(s) on the model(s). Called from main.cpp.
Additional Inherited Members

13.51.1 Detailed Description

Environment corresponding to execution as a stand-alone application.

This environment corresponds to a stand-alone executable program, e.g., main.cpp. It sets up the Parallel-Library, ProgramOptions, and ProblemDescDB objects based on access to command line arguments.

The documentation for this class was generated from the following files:

- ExecutableEnvironment.hpp
- ExecutableEnvironment.cpp

13.52 ExperimentData Class Reference

Interpolation method for interpolating between experimental and model data. I need to work on inputs/outputs to this method. For now, this assumes interpolation of functional data.

Public Member Functions

- **ExperimentData ()**
  default constructor

- **ExperimentData (const ProblemDescDB &prob_desc_db, const SharedResponseData &srd, short output_level)**
  typical DB-based constructor

- **ExperimentData (size_t num_experiments, size_t num_config_vars, const boost::filesystem::path &data_prefix, const SharedResponseData &srd, const StringArray &variance_types, short output_level, std::string scalarDataFilename="")**
  temporary? constructor for testing

- **ExperimentData (size_t num_experiments, const SharedResponseData &srd, const RealMatrix &configVars, const IntResponseMap &all_responses, short output_level)**

- **void load_data (const std::string &context_message)**
  Load experiments from data files (simple scalar or field)

- **void add_data (const RealVector &one_configvars, const Response &one_response)**
  Add one data point to the experimental data set.

- **size_t num_experiments () const**
  retrieve the number of experiments

- **size_t num_total_exppoints () const**
  retrieve the total number of experimental data points over all experiments

- **size_t num_scalars () const**
  retrieve the number of scalars (applies to all experiments)

- **size_t num_fields () const**
  retrieve the number of fields (applies to all experiments)

- **size_t num_config_vars () const**
  number of configuration variables

- **const std::vector< RealVector > & config_vars () const**
  values of the configuration variables, 1 RealVector per experiment
• const RealVector & all_data (size_t experiment)
  return contiguous vector of all data (scalar, followed by field) for the specified experiment
• const Response & response (size_t experiment)
  return response for the specified experiment
• void per_exp_length (IntVector &per_length) const
  return the individual sizes of the experimental data lengths (all function values, scalar and field)
• const IntVector & field_lengths (size_t experiment) const
  return the field lengths for the specified experiment index
• Real scalar_data (size_t response, size_t experiment)
  retrieve the data value for the given response, for the given experiment
• RealVector field_data_view (size_t response, size_t experiment) const
  retrieve a view of the field data for the given response, for the given experiment
• RealMatrix field_coords_view (size_t response, size_t experiment) const
  retrieve a view of the field data coordinates for the given response, for the given experiment
• bool variance_type_active (short variance_type) const
  whether the specified variance type (enum value) is present and active
• bool variance_active () const
  whether any variance type is active
• Real apply_covariance (const RealVector &residuals, size_t experiment) const
  apply the covariance responses to compute the triple product $v^* \cdot \text{inv}(C) \cdot v$ for the given experiment
• void apply_covariance_inv_sqrt (const RealVector &residuals, size_t experiment, RealVector &weighted_residuals) const
  apply inverse sqrt of the covariance to compute weighted residuals
• void apply_covariance_inv_sqrt (const RealMatrix &gradients, size_t experiment, RealMatrix &weighted_gradients) const
  apply inverse sqrt of the covariance to compute weighted gradients
• void apply_covariance_inv_sqrt (const RealSymMatrixArray &hessians, size_t experiment, RealSymMatrixArray &weighted_hessians) const
  apply inverse sqrt of the covariance to compute weighted Hessians
• void get_main_diagonal (RealVector &diagonal, size_t experiment) const
  return a (copy) vector containing the main diagonal entries of a specified experimental covariance matrix
• void cov_std_deviation (RealVectorArray &std_deviation) const
  get the standard deviation of the observation error process, one vector per experiment
• void cov_as_correlation (RealSymMatrixArray &corr_matrix) const
  get the observation error covariance as a correlation matrix, one vector per experiment
• void covariance (int exp_ind, RealSymMatrix &cov_mat) const
  retrieve an individual covariance entry as a dense matrix
• void form_residuals (const Response &sim_resp, Response &residual Resp) const
  form residuals for all experiments, interpolating if necessary; one simulation response maps to all experiments
• void form_residuals (const Response &sim_resp, const size_t curr_exp, Response &residual Resp) const
  Populate the portion of residual Resp corresponding to experiment curr_exp; the passed simulation response maps only to the specified experiment.
• void form_residuals (const Response &sim_resp, size_t exp_num, const ShortArray &total_asv, size_t residual Resp_offset, Response &residual Resp) const
form residuals for an individual experiment, interpolating if necessary

- **void recover_model** (size_t num_pri_fns, RealVector &model_fns) const
  recover original model from the first experiment block in a full set of residuals; works in no interpolation case only (sizes same)

- **bool interpolate_flag** () const
  flag for interpolation. If 0, no interpolation. If 1, interpolate.

- **void interpolate_simulation_data** (const Response &sim_resp, size_t exp_num, const ShortArray &total_asv, size_t exp_offset, Response &interp_resp) const
  Interpolate simulation data (values, gradients and hessians) onto the coordinates of the experimental data.

- **void scale_residuals** (const Response &residual_response, RealVector &scaled_residuals) const
  Apply the experiment data covariance to the residual data (scale functions by $\Gamma_d^{-1/2}$), returning in scaled_residuals.

- **void scale_residuals** (Response &residual_response) const
  Apply the experiment data covariance to the residual data in-place (scale functions, gradients, and Hessians by $\Gamma_d^{-1/2}$)

- **void build_gradient_of_sum_square_residuals** (const Response &resp, RealVector &ssr_gradient) const
  Build the gradient of the ssr from residuals and function gradients based on the response’s active set request vector.

- **void build_gradient_of_sum_square_residuals** (const Response &resp, const ShortArray &asrv, RealVector &ssr_gradient) const
  Build the gradient of the ssr from residuals and function gradients using the passed active set request vector (overrides the response’s request vector)

- **void build_gradient_of_sum_square_residuals_from_response** (const Response &resp, const ShortArray &asrv, int exp_ind, RealVector &ssr_gradient) const
  Update the gradient of ssr with the values from the gradient associated with a single experiment.

- **void build_gradient_of_sum_square_residuals_from_function_data** (const RealMatrix &func_gradients, const RealVector &residuals, RealVector &ssr_gradient) const
  Construct the gradient of the sum of squares of residuals.

- **void build_hessian_of_sum_square_residuals** (const Response &resp, RealSymMatrix &ssr_hessian) const
  Build the hessian of the ssr from residuals, function gradients and function Hessians based on the response’s active set request vector.

- **void build_hessian_of_sum_square_residuals** (const Response &resp, const ShortArray &asrv, RealSymMatrix &ssr_hessian) const
  Build the hessian of the ssr from residuals, function gradients and function Hessians using the passed active set request vector (overrides the response’s request vector)

- **void build_hessian_of_sum_square_residuals_from_response** (const Response &resp, const ShortArray &asrv, int exp_ind, RealSymMatrix &ssr_hessian) const
  Update the hessian of ssr with the values from the hessian associated with a single experiment.

- **void build_hessian_of_sum_square_residuals_from_function_data** (const RealSymMatrixArray &func_hessians, const RealMatrix &func_gradients, const RealVector &residuals, RealSymMatrix &ssr_hessian, const ShortArray &asrv) const
  Construct the hessian of the sum of squares of residuals.

- **void scale_residuals** (const RealVector &multipliers, unsigned short multiplier_mode, size_t num_calib_params, Response &residual_response) const
  In-place scale the residual response (functions, gradients, Hessians) by $\sqrt{\text{multipliers}}$, according to blocks indicated by multiplier_mode

- **Real cov_determinant** (const RealVector &multipliers, unsigned short multiplier_mode) const
returns the determinant of (covariance block-scaled by the passed multipliers)

- Real `half_log_cov_determinant` (const RealVector &multipliers, unsigned short multiplier_mode) const
  returns the log of the determinant of (covariance block-scaled by the passed multipliers)
- void `half_log_cov_det_gradient` (const RealVector &multipliers, unsigned short multiplier_mode, size_t hyper_offset, RealVector &gradient) const
  populated the passed gradient with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)
- void `half_log_cov_det_hessian` (const RealVector &multipliers, unsigned short multiplier_mode, size_t hyper_offset, RealSymMatrix &hessian) const
  populated the passed Hessian with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)
- StringArray `hyperparam_labels` (unsigned short multiplier_mode) const
  generate variable labels for the covariance (error) multiplier hyperparams

Protected Member Functions

- ShortArray `determine_active_request` (const Response &resid_resp) const
  Perform check on the active request vector to make sure it is amenable to interpolation of simulation data and application of apply covariance.
- SizetArray `residuals_per_multiplier` (unsigned short multiplier_mode) const
  count the number of residuals influenced by each multiplier
- void `generate_multipliers` (const RealVector &multipliers, unsigned short multiplier_mode, RealVector &expanded_multipliers) const
  Generate a set of multipliers commensurate with the residual size for the total experiment data set. Instead of repeating the loops all over the place, generate an expanded set of multipliers; the conditionals get too complicated otherwise.
- void `resid2mult_map` (unsigned short multiplier_mode, IntVector &resid2mult_indices) const
  return the index of the multiplier that affects each residual

Private Member Functions

- void `initialize` (const StringArray &variance_types, const SharedResponseData &srd)
  shared body of constructor initialization
- void `parse_sigma_types` (const StringArray &sigma_types)
  parse user-provided sigma type strings and populate enums
- void `load_experiment` (size_t exp_index, std::ifstream &scalar_data_stream, size_t num_field_sigma_matrices, size_t num_field_sigma_diagonals, size_t num_field_sigma_scalars, size_t num_field_sigma_none, Response &exp_resp)
  Load a single experiment exp_index into exp_resp.
- void `read_scalar_sigma` (std::ifstream &scalar_data_stream, RealVector &sigma_scalars, IntVector &scalar_map_indices)
  read or default populate the scalar sigma
- RealVector `residuals_view` (const RealVector &residuals, size_t experiment) const
  Return a view (to allowing updating in place) of the residuals associated with a given experiment, from a vector containing residuals from all experiments.
- RealMatrix `gradients_view` (const RealMatrix &gradients, size_t experiment) const
Return a view (to allowing updating in place) of the gradients associated with a given experiment, from a matrix containing gradients from all experiments.

- **RealSymMatrixArray** `hessians_view` (const RealSymMatrixArray &hessians, size_t experiment) const
  
  Return a view (to allowing updating in place) of the hessians associated with a given experiment, from an array containing the hessians from all experiments.

### Private Attributes

- **bool** `calibrationDataFlag`
  
  whether the user specified a calibration data block

- **size_t** `numExperiments`
  
  the total number of experiments

- **size_t** `numConfigVars`
  
  number of configuration (state) variables to read for each experiment

- **UShortArray** `varianceTypes`
  
  type of variance specified for each variable, one per response group; empty varianceType indicates none specified by user

- **Real** `covarianceDeterminant`
  
  cached product of each experiment covariance’s determinant

- **Real** `logCovarianceDeterminant`
  
  cached sum of each experiment covariance’s log determinant

- **boost::filesystem::path** `dataPathPrefix`
  
  path to prepend to any data file names

- **String** `scalarDataFilename`
  
  the user-specified scalar data filename

- **unsigned short** `scalarDataFormat`
  
  tabular format of the simple scalar data file; supports TABULAR_NONE, TABULAR_HEADER, TABULAR_EVAL_ID, TABULAR_EXPER_ANNOT

- **size_t** `scalarSigmaPerRow`
  
  number of sigma values to read from each row in simple data file format (calculated from variance types strings

- **bool** `readSimFieldCoords`
  
  whether to read coordinate data files for simulation fields

- **SharedResponseData** `simulationSRD`
  
  archived shared data for use in sizing fields, total functions (historically we read all functions, including constraints, which might not be correct)

- **bool** `interpolateFlag`
  
  flag for interpolation.

- **short** `outputLevel`
  
  output verbosity level

- **std::vector< Response >** `allExperiments`
  
  Vector of numExperiments ExperimentResponses, holding the observed data and error (sigma/covariance) for each experiment.

- **std::vector< RealVector >** `allConfigVars`
  
  Vector of numExperiments configurations at which data were gathered; empty if no configurations specified.

- **IntVector** `experimentLengths`
13.52. EXPERIMENTDATA CLASS REFERENCE

Length of each experiment.

- IntVector expOffsets
  function index offsets for individual experiment data sets

13.52.1 Detailed Description

Interpolation method for interpolating between experimental and model data. I need to work on inputs/outputs to this method. For now, this assumes interpolation of functional data.

As Brian suggested, this class has the experimental data (coordinates and RealVectorArray interpolated-Results; The ExperimentData class is used to read and populate data (currently from user-specified files and/or the input spec) relating to experimental (physical observations) data for the purposes of calibration. Such data may include (for example): number of experiments, configuration variables, type of data (scalar vs. functional), treatment of sigma (experimental uncertainties). This class also provides an interpolation capability to interpolate between simulation or experimental data so that the differencing between simulation and experimental data may be performed properly.

13.52.2 Member Function Documentation

**void form_residuals** ( const Response & sim_resp, Response & residual_resp ) const

form residuals for all experiments, interpolating if necessary; one simulation response maps to all experiments

This assumes the source gradient/Hessian are size less or equal to the destination response, and that the leading part is to be populated.

References ExperimentData::determine_active_request(), ExperimentData::numExperiments, and ExperimentData::per_exp_length().

Referenced by DataTransformModel::derived_evaluate(), ExperimentData::form_residuals(), DataTransformModel::primary_resp_differencer(), and DataTransformModel::transform_response_map().

**void form_residuals** ( const Response & sim_resp, size_t exp_ind, const ShortArray & total_asv, size_t exp_offset, Response & residual_resp ) const

form residuals for an individual experiment, interpolating if necessary

This assumes the source gradient/Hessian are size less or equal to the destination response, and that the leading part is to be populated.

References ExperimentData::allExperiments, ExperimentData::field_data_view(), Response::field_lengths(), Response::function_gradient_view(), Response::function_gradients(), Response::function_gradients_view(), Response::function_hessian_view(), Response::function_hessians(), Response::function_hessians_view(), Response::function_values(), Response::function_values_view(), ExperimentData::gradients_view(), ExperimentData::hessians_view(), ExperimentData::interpolate_simulation_data(), ExperimentData::interpolateFlag, ExperimentData::num_fields(), ExperimentData::num_scalars(), and ExperimentData::outputLevel.

**void recover_model** ( size_t num_pri_fns, RealVector & best_fns ) const

recover original model from the first experiment block in a full set of residuals; works in no interpolation case only (sizes same)

Add the data back to the residual to recover the model, for use in surrogated-based LSQ where DB lookup will fail (need approx eval DB). best_fns contains primary and secondary responses

References Dakota::abort_handler(), ExperimentData::allExperiments, Response::function_value(), ExperimentData::interpolateFlag, and Response::num_functions().

Referenced by LeastSq::post_run().
void build_gradient_of_sum_square_residuals_from_function_data ( const RealMatrix & func_gradients, const RealVector & residuals, RealVector & ssr_gradient, const ShortArray & asrv )

Construct the gradient of the sum of squares of residuals.
Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>func_gradients</code></td>
<td>A matrix containing the gradients of the residual vector</td>
</tr>
<tr>
<td><code>residuals</code></td>
<td>A vector of residuals (mismatch between experimental data and the corresponding function values)</td>
</tr>
<tr>
<td><code>asrv</code></td>
<td>The active set request vector</td>
</tr>
</tbody>
</table>

Referenced by ExperimentData::build_gradient_of_sum_square_residuals_from_response().

```cpp
void build_hessian_of_sum_square_residuals_from_function_data ( const RealSymMatrixArray & func_hessians, const RealMatrix & func_gradients, const RealVector & residuals, RealSymMatrix & ssr_hessian, const ShortArray & asrv )
```

Construct the hessian of the sum of squares of residuals.

Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>func_hessians</code></td>
<td>A list of matrices containing the Hessians of the function elements in the residual vector</td>
</tr>
<tr>
<td><code>func_gradients</code></td>
<td>A matrix containing the gradients of the residual vector</td>
</tr>
<tr>
<td><code>residuals</code></td>
<td>A vector of residuals (mismatch between experimental data and the corresponding function values)</td>
</tr>
<tr>
<td><code>asrv</code></td>
<td>The active set request vector</td>
</tr>
</tbody>
</table>

Referenced by ExperimentData::build_hessian_of_sum_square_residuals_from_response().

```cpp
void scale_residuals ( const RealVector & multipliers, unsigned short multiplier_mode, size_t num_calib_params, Response & residual_response ) const
```

in-place scale the residual response (functions, gradients, Hessians) by sqrt(multipliers), according to blocks indicated by multiplier mode

- In-place scaling of residual response by hyper-parameter multipliers
- References Dakota::abort_handler(), Response::active_set_request_vector(), Response::function_gradient_view(), Response::function_hessian_view(), Response::function_value(), Response::function_value_view(), ExperimentData::num_total_exppoints(), and ExperimentData::resid2mult_map().

```cpp
Real cov_determinant ( const RealVector & multipliers, unsigned short multiplier_mode ) const
```

returns the determinant of (covariance block-scaled by the passed multipliers)

- Determinant of the total covariance used in inference, which has blocks $\text{mult}_i \cdot I \cdot \text{Cov}_i$.
- References Dakota::abort_handler(), ExperimentData::covarianceDeterminant, ExperimentData::generate_multipliers(), and ExperimentData::num_total_exppoints().

```cpp
Real half_log_cov_determinant ( const RealVector & multipliers, unsigned short multiplier_mode ) const
```

returns the log of the determinant of (covariance block-scaled by the passed multipliers)

- Determinant of half the log of total covariance used in inference, which has blocks $\text{mult}_i \cdot I \cdot \text{Cov}_i$.
- References Dakota::abort_handler(), ExperimentData::generate_multipliers(), ExperimentData::logCovarianceDeterminant, and ExperimentData::num_total_exppoints().
- Referenced by NonDBayesCalibration::log_likelihood(), and NonDQUESOBayesCalibration::print_results().
void half_log_cov_det_gradient ( const RealVector & multipliers, unsigned short multiplier_mode, size_t hyper_offset, RealVector & gradient ) const

populated the passed gradient with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)
  Compute the gradient of scalar \( f(m) = 0.5 \cdot \log(\det(m \cdot \text{Cov})) \) w.r.t. mults. Since this is the only use case, we include the 0.5 factor and perform an update in-place.
  References ExperimentData::num_total_exppoints(), and ExperimentData::residuals_per_multiplier().
  Referenced by NonDBayesCalibration::neg_log_post_resp_mapping().

void half_log_cov_det_hessian ( const RealVector & multipliers, unsigned short multiplier_mode, size_t hyper_offset, RealSymMatrix & hessian ) const

populated the passed Hessian with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)
  Compute the gradient of scalar \( f(m) = \log(\det(m \cdot \text{Cov})) \) w.r.t. mults
  References ExperimentData::num_total_exppoints(), and ExperimentData::residuals_per_multiplier().
  Referenced by NonDBayesCalibration::neg_log_post_resp_mapping().

SizetArray residuals_per_multiplier ( unsigned short multiplier_mode ) const [protected]

count the number of residuals influenced by each multiplier
  Calculate how many residuals each multiplier affects
  References ExperimentData::allExperiments, SharedResponseData::num_field_response_groups(), ExperimentData::num_fields(), SharedResponseData::num_response_groups(), SharedResponseData::num_scalar_responses(), ExperimentData::numExperiments, and ExperimentData::simulationSRD.
  Referenced by ExperimentData::half_log_cov_det_gradient(), and ExperimentData::half_log_cov_det_hessian().

void parse_sigma_types ( const StringArray & sigma_types ) [private]

parse user-provided sigma type strings and populate enums
  Validate user-provided sigma specification. User can specify 0, 1, or num_response_groups sigmas. If specified, sigma types must be the same for all scalar responses.
  References Dakota::abort_handler(), SharedResponseData::num_response_groups(), SharedResponseData::num_scalar_responses(), ExperimentData::scalarDataFilename, ExperimentData::scalarSigmaPerRow, ExperimentData::simulationSRD, and ExperimentData::varianceTypes.
  Referenced by ExperimentData::initialize().

void load_experiment ( size_t exp_index, std::ifstream & scalar_data_stream, size_t num_field_sigma_matrices, size_t num_field_sigma_diagonals, size_t num_field_sigma_scalars, size_t num_field_sigma_none, Response & exp.resp ) [private]

Load a single experiment exp_index into exp.resp.
  Load an experiment from a mixture of legacy format data and field data format files
  References Dakota::abort_handler(), ExperimentData::dataPathPrefix, Response::field_coords(), Response::field_group_labels(), ExperimentData::field_lengths(), Response::field_lengths(), Response::field_values(), Response::function_labels(), Response::function_value(), Dakota::is_matrix_symmetric(), SharedResponseData::num_field_response_groups(), ExperimentData::num_fields(), SharedResponseData::num_scalar_responses(), ExperimentData::num_scalars(), ExperimentData::read_scalar_sigma(), ExperimentData::scalarDataFilename, ExperimentData::scalarSigmaPerRow, Response::set_full_covariance(), ExperimentData::simulationSRD, and ExperimentData::varianceTypes.
13.53 EXPERIMENTRESPONSE CLASS REFERENCE

Referenced by ExperimentData::load_data().
The documentation for this class was generated from the following files:

- ExperimentData.hpp
- ExperimentData.cpp

13.53 ExperimentResponse Class Reference

Container class for response functions and their derivatives. ExperimentResponse provides the body class.

Inheritance diagram for ExperimentResponse:

```
<table>
<thead>
<tr>
<th>Response</th>
</tr>
</thead>
<tbody>
<tr>
<td>ExperimentResponse</td>
</tr>
</tbody>
</table>
```

Public Member Functions

- **ExperimentResponse ()**
  default constructor
- **ExperimentResponse (const Variables &vars, const ProblemDescDB &problem_db)**
  standard constructor built from problem description database
- **ExperimentResponse (const SharedResponseData &srd, const ActiveSet &set)**
  alternate constructor that shares a SharedResponseData instance
- **ExperimentResponse (const SharedResponseData &srd)**
  alternate constructor that shares a SharedResponseData instance
- **ExperimentResponse (const ActiveSet &set)**
  alternate constructor using limited data
- **~ExperimentResponse ()**
  destructor
- **void set_scalar_covariance (RealVector &scalars)**
  method to set the covariance matrix defined for ExperimentResponse
- **const ExperimentCovariance & experiment_covariance () const**
  retrieve the ExperimentCovariance structure
- **void set_full_covariance (std::vector< RealMatrix > &matrices, std::vector< RealVector > &diagonals, RealVector &scalars, IntVector matrix_map_indices, IntVector diagonal_map_indices, IntVector scalar_map_indices)**
  method to set the full covariance matrices for ExperimentResponse
- **Real apply_covariance (const RealVector &residual) const**
  method to compute the triple product $v'\cdot \text{inv}(C) \cdot v$
- **void apply_covariance_inv_sqrt (const RealVector &residuals, RealVector &weighted_residuals) const**
  method to compute $(v'\cdot \text{inv}(C) \cdot 1/2)_i$, to compute weighted residual
- **void apply_covariance_inv_sqrt (const RealMatrix &gradients, RealMatrix &weighted_gradients) const**
• void **apply_covariance_inv_sqrt** (const RealSymMatrixArray &hessians, RealSymMatrixArray &weighted_hessians) const
• void **get_covariance_diagonal** (RealVector &diagonal) const
• Real **covariance_determinant** () const
  
  covariance determinant for this experiment (default 1.0)
• Real **log_covariance_determinant** () const
  
  log covariance determinant for this experiment (default 0.0)

Protected Member Functions

• void **copy_rep** (Response *source RESP_rep)
  
  Specialization of copy_rep; pulls base class data as well as derived specific data from the source rep into the this object.

Private Attributes

• ExperimentCovariance **expDataCovariance**
  sigma terms...

Additional Inherited Members

13.53.1 Detailed Description

Container class for response functions and their derivatives. **ExperimentResponse** provides the body class.

The **ExperimentResponse** class is the "representation" of the response container class. It is the "body" portion of the "handle-body idiom" (see Coplien "Advanced C++", p. 58). The handle class (**Response**) provides for memory efficiency in management of multiple response objects through reference counting and representation sharing. The body class (**ExperimentResponse**) actually contains the response data (functionValues, function-Gradients, functionHessians, etc.). The representation is hidden in that an instance of **ExperimentResponse** may only be created by **Response**. Therefore, programmers create instances of the **Response** handle class, and only need to be aware of the handle/body mechanisms when it comes to managing shallow copies (shared representation) versus deep copies (separate representation used for history mechanisms).

The documentation for this class was generated from the following files:

• **ExperimentResponse.hpp**
• **ExperimentResponse.cpp**

13.54 FileReadException Class Reference

base class for Dakota file read exceptions (to allow catching both tabular and general file truncation issues)

Inheritance diagram for FileReadException:

```
FileReadException
  
ResultsFileError   TabularDataTruncated
```
### 13.55. FORKAPPLICINTERFACE CLASS REFERENCE

**Public Member Functions**

- `FileReadException (const std::string &msg)`

**13.54.1 Detailed Description**

Base class for Dakota file read exceptions (to allow catching both tabular and general file truncation issues). The documentation for this class was generated from the following file:

- dakota_global_defs.hpp

### 13.55 ForkApplicInterface Class Reference

Derived application interface class which spawns simulation codes using fork/execvp/waitpid.

Inheritance diagram for ForkApplicInterface:

```
+-----------------+            +-----------------+            +-----------------+            +-----------------+
| Interface       |            | ApplicationInterface |            | ProcessApplicInterface |            | ProcessHandleApplicInterface |
|                 |            |                      |            |                       |            |                             |
| ForkApplicInterface |          |                      |            |                       |            |                             |
```

**Public Member Functions**

- `ForkApplicInterface (const ProblemDescDB &problem_db)`
  
  Constructor
  
- `~ForkApplicInterface ()`
  
  Destructor

**Protected Member Functions**

- `void wait_local_evaluations (PRPQueue &prp_queue)`
  
  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.

- `void test_local_evaluations (PRPQueue &prp_queue)`
  
  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version is nonblocking and will return without any completions if none are immediately available.

- `pid_t create_analysis_process (bool block_flag, bool new_group)`
  
  Spawn a child process for an analysis component within an evaluation using fork()/execvp() and wait for completion using waitpid() if block_flag is true.
• size_t wait_local_analyses ()
  wait for asynchronous analyses on the local processor; completing at least one job
• size_t test_local_analyses_send (int analysis_id)
  test for asynchronous analysis completions on the local processor and return results for any completions by sending messages
• void join_evaluation_process_group (bool new_group)
  create (if new_group) and join the process group for async evaluations
• void join_analysis_process_group (bool new_group)
  create (if new_group) and join the process group for async analyses
• void evaluation_process_group_id (pid_t pgid)
  set evalProcGroupId
• pid_t evaluation_process_group_id () const
  return evalProcGroupId
• void analysis_process_group_id (pid_t pgid)
  set analysisProcGroupId
• pid_t analysis_process_group_id () const
  return analysisProcGroupId
• pid_t wait_evaluation (bool block_flag)
  process all available completions within the evaluation process group; if block_flag = true, wait for at least one completion
• pid_t wait_analysis (bool block_flag)
  process all available completions within the analysis process group; if block_flag = true, wait for at least one completion
• void check_group (int err, pid_t proc_group_id)
  check the exit status of setpgid and abort if an error code was returned

Private Member Functions

• pid_t wait (pid_t proc_group_id, std::map< pid_t, int >&process_id_map, bool block_flag)
  core code used by wait_{evaluation,analysis}()
• void join_process_group (pid_t &process_group_id, bool new_group)
  core code used by join_{evaluation,analysis}.process_group()

Private Attributes

• pid_t evalProcGroupId
  the process group id used to identify a set of child evaluation processes used by this interface instance (to distinguish from other interface instances that could be running at the same time)
• pid_t analysisProcGroupId
  the process group id used to identify a set of child analysis processes used by this interface instance (to distinguish from other interface instances that could be running at the same time)
13.56. **FSUDESIGNCOMPEXP CLASS REFERENCE**

**Additional Inherited Members**

**13.55.1 Detailed Description**

Derived application interface class which spawns simulation codes using fork/execvp/waitpid. 

ForkApplicInterface is used on Unix systems and is a peer to SpawnApplicInterface for Windows systems. 

The documentation for this class was generated from the following files:

- ForkApplicInterface.hpp
- ForkApplicInterface.cpp

**13.56 FSUDesignCompExp Class Reference**

Wrapper class for the FSUDace QMC/CVT library.

Inheritance diagram for FSUDesignCompExp:

```
  FSUDesignCompExp
    |                        |
    v                        v
  PStudyDACE
    |                        |
    v                        v
  Analyzer
    |                        |
    v                        v
  Iterator
```

**Public Member Functions**

- FSUDesignCompExp (ProblemDescDB &problem_db, Model &model)  
  primary constructor for building a standard DACE iterator
- FSUDesignCompExp (Model &model, int samples, int seed, unsigned short sampling::method)  
  alternate constructor for building a DACE iterator on-the-fly
- ~FSUDesignCompExp ()  
  destructor
- bool resize ()  
  reinitializes iterator based on new variable size

**Protected Member Functions**

- void pre_run ()  
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()  
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void post_input ()  
  read tabular data for post-run mode
CHAPTER 13. CLASS DOCUMENTATION

- void `post_run` (std::ostream &s)
  
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

- int `num_samples` () const

- void `sampling_reset` (int min_samples, bool all_data_flag, bool stats_flag)
  
  reset sampling iterator to use at least min_samples

- unsigned short `sampling_scheme` () const
  
  return sampling name

- void `vary_pattern` (bool pattern_flag)
  
  sets varyPattern in derived classes that support it

- void `get_parameter_sets` (Model &model)
  
  Generate one block of numSamples samples (ndim * num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.

- void `get_parameter_sets` (Model &model, const int num_samples, RealMatrix &design_matrix)
  
  Generate one block of numSamples samples (ndim * num_samples), populating design_matrix.

Private Member Functions

- void `enforce_input_rules` ()
  
  enforce sanity checks/modifications for the user input specification

Private Attributes

- int `samplesSpec`
  
  initial specification of number of samples

- int `numSamples`
  
  current number of samples to be evaluated

- bool `allDataFlag`
  
  flag which triggers the update of allVars/allResponses for use by Iterator::all_variables() and Iterator::all_responses()

- size_t `numDACERuns`
  
  counter for number of executions for this object

- bool `latinizeFlag`
  
  flag which specifies latinization of QMC or CVT sample sets

- IntVector `sequenceStart`
  
  Integer vector defining a starting index into the sequence for random variable sampled. Default is 0 0 0 (e.g. for three random variables).

- IntVector `sequenceLeap`
  
  Integer vector defining the leap number for each sequence being generated. Default is 1 1 1 (e.g. for three random vars.)

- IntVector `primeBase`
  
  Integer vector defining the prime base for each sequence being generated. Default is 2 3 5 (e.g., for three random vars.)

- int `seedSpec`
  
  the user seed specification for the random number generator (allows repeatable results)

- int `randomSeed`
current seed for the random number generator

- **bool varyPattern**
  
  flag for continuing the random number or QMC sequence from a previous execution (e.g., for surrogate-based optimization) so that multiple executions are repeatable but not identical.

- **int numCVTTrials**

  specifies the number of sample points taken at internal CVT iteration

- **int trialType**

  Trial type in CVT. Specifies where the points are placed for consideration relative to the centroids. Choices are grid (2), halton (1), uniform (0), or random (-1). Default is random.

**Additional Inherited Members**

**13.56.1 Detailed Description**

Wrapper class for the FSUDace QMC/CVT library.

The FSUDesignCompExp class provides a wrapper for FSUDace, a C++ design of experiments library from Florida State University. This class uses quasi Monte Carlo (QMC) and Centroidal Voronoi Tesselation (CVT) methods to uniformly sample the parameter space spanned by the active bounds of the current Model. It returns all generated samples and their corresponding responses as well as the best sample found.

**13.56.2 Constructor & Destructor Documentation**

**FSUDesignCompExp ( ProblemDescDB & problem_db, Model & model )**

primary constructor for building a standard DACE iterator

This constructor is called for a standard iterator built with data from probDescDB.

References Dakota::abort_handler(), ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_iv(), ProblemDescDB::get_string(), Iterator::maxEvalConcurrency, Iterator::methodName, Analyzer::numContinuousVars, FSUDesignCompExp::numCVTTrials, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, FSUDesignCompExp::numSamples, FSUDesignCompExp::primeBase, Iterator::probDescDB, FSUDesignCompExp::randomSeed, FSUDesignCompExp::seedSpec, FSUDesignCompExp::sequenceLeap, FSUDesignCompExp::sequenceStart, and FSUDesignCompExp::trialType, and FSUDesignCompExp::varyPattern.

**FSUDesignCompExp ( Model & model, int samples, int seed, unsigned short sampling_method )**

alternate constructor for building a DACE iterator on-the-fly

This alternate constructor is used for instantiations on-the-fly, using only the incoming data. No problem description database queries are used.

References Dakota::abort_handler(), Iterator::maxEvalConcurrency, Iterator::methodName, Analyzer::numContinuousVars, FSUDesignCompExp::numCVTTrials, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, FSUDesignCompExp::numSamples, FSUDesignCompExp::primeBase, FSUDesignCompExp::randomSeed, FSUDesignCompExp::seedSpec, FSUDesignCompExp::sequenceLeap, FSUDesignCompExp::sequenceStart, and FSUDesignCompExp::trialType.

**13.56.3 Member Function Documentation**

**void pre_run ( ) [protected], [virtual]**

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s \texttt{pre\_run()}, if implemented, typically \textit{before} performing its own implementation steps.

Reimplemented from \texttt{Analyzer}.

References \texttt{FSUDesignCompExp::enforce\_input\_rules()}, \texttt{FSUDesignCompExp::get\_parameter\_sets()}, \texttt{Analyzer::get\_vbd\_parameter\_sets()}, \texttt{Analyzer::iteratedModel}, \texttt{FSUDesignCompExp::num\_Samples}, \texttt{Analyzer::pre\_run()}, and \texttt{PStudyDACE::var\_Based\_Decomp\_Flag}.

\texttt{void core\_run\() [protected], [virtual]}

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from \texttt{Iterator}.

References \texttt{FSUDesignCompExp::all\_Data\_Flag}, \texttt{Analyzer::evaluate\_parameter\_sets()}, \texttt{Analyzer::iteratedModel}, \texttt{Analyzer::num\_LSq\_Terms}, \texttt{Analyzer::num\_Obj\_Fns}, and \texttt{Analyzer::post\_run()}.

\texttt{void post\_run\() \texttt{( std::ostream } & s) [protected], [virtual]}

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s \texttt{post\_run()}, typically \textit{after} performing its own implementation steps.

Reimplemented from \texttt{Analyzer}.

References \texttt{Analyzer::all\_Responses}, \texttt{Analyzer::all\_Samples}, \texttt{Sens\_Analysis\_Global::compute\_correlations()}, \texttt{Analyzer::compute\_vbd\_stats()}, \texttt{FSUDesignCompExp::enforce\_input\_rules()}, \texttt{FSUDesignCompExp::num\_Samples}, \texttt{Analyzer::post\_run()}, \texttt{PStudyDACE::p\_Study\_DACE\_Sens\_Global}, \texttt{Analyzer::sub\_Iterator\_Flag}, and \texttt{PStudyDACE::var\_Based\_Decomp\_Flag}.

\texttt{int num\_samples\() const [inline], [protected], [virtual]}

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the max\_Eval\_Concurrency.

Reimplemented from \texttt{Analyzer}.

References \texttt{FSUDesignCompExp::num\_Samples}.

Referenced by \texttt{FSUDesignCompExp::get\_parameter\_sets}().

\texttt{void enforce\_input\_rules\() [private]}

enforce sanity checks/modifications for the user input specification.

Users may input a variety of quantities, but this function must enforce any restrictions imposed by the sampling algorithms.

References \texttt{Dakota::abort\_handler()}, \texttt{Analyzer::method\_Name}, \texttt{Analyzer::num\_Continuous\_Vars}, \texttt{FSUDesign\_Comp\_Exp::num\_Samples}, and \texttt{FSUDesign\_Comp\_Exp::prime\_Base}.

Referenced by \texttt{FSUDesign\_Comp\_Exp::post\_input()}, \texttt{FSUDesign\_Comp\_Exp::post\_run()}, and \texttt{FSUDesign\_Comp\_Exp::pre\_run()}.

The documentation for this class was generated from the following files:

- \texttt{FSUDesign\_Comp\_Exp\_hpp}
- \texttt{FSUDesign\_Comp\_Exp\_cpp}
13.57 FunctionEvalFailure Class Reference

Exception class for function evaluation failures
Inherits runtime_error.

Public Member Functions

- FunctionEvalFailure (const std::string &msg)

13.57.1 Detailed Description

Exception class for function evaluation failures
The documentation for this class was generated from the following file:
- dakota.global_defs.hpp

13.58 GaussProcApproximation Class Reference

Derived approximation class for Gaussian Process implementation.
Inheritance diagram for GaussProcApproximation:

```
      Approximation
       |          |
       | GaussProcApproximation
```

Public Member Functions

- GaussProcApproximation ()
  default constructor
- GaussProcApproximation (const SharedApproxData &shared_data)
  alternate constructor
- GaussProcApproximation (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)
  standard constructor
- ~GaussProcApproximation ()
  destructor

Protected Member Functions

- int min_coefficients () const
  return the minimum number of samples (unknowns) required to build the derived class approximation type in num-Vars dimensions
- int num_constraints () const
  return the number of constraints to be enforced via an anchor point
- void build ()
find the covariance parameters governing the Gaussian process response

- **Real value** (const Variables &vars)
  retrieve the function value for a given parameter set
- **const RealVector & gradient** (const Variables &vars)
  retrieve the function gradient at the predicted value for a given parameter set
- **Real prediction_variance** (const Variables &vars)
  retrieve the variance of the predicted value for a given parameter set

### Private Member Functions

- **void GPmodel_build ()**
  Function to compute hyperparameters governing the GP.
- **void GPmodel_apply (const RealVector &new_x, bool variance_flag, bool gradients_flag)**
  Function returns a response value using the GP surface.
- **void normalize_training_data ()**
  Normalizes the initial inputs upon which the GP surface is based.
- **void get_trend ()**
  Gets the trend (basis) functions for the calculation of the mean of the GP. If the order = 0, the trend is a constant, if the order = 1, trend is linear, if order = 2, trend is quadratic.
- **void get_beta_coefficients ()**
  Gets the beta coefficients for the calculation of the mean of the GP.
- **int get_cholesky_factor ()**
  Gets the Cholesky factorization of the covariance matrix, with error checking.
- **void get_process_variance ()**
  Gets the estimate of the process variance given the values of beta and the correlation lengthscales.
- **void get_cov_matrix ()**
  calculates the covariance matrix for a given set of input points
- **void get_cov_vector ()**
  calculates the covariance vector between a new point x and the set of inputs upon which the GP is based
- **void optimize_theta_global ()**
  sets up and performs the optimization of the negative log likelihood to determine the optimal values of the covariance parameters using NCSUDirect
- **void optimize_theta_multipoint ()**
  sets up and performs the optimization of the negative log likelihood to determine the optimal values of the covariance parameters using a gradient-based solver and multiple starting points
- **void predict (bool variance_flag, bool gradients_flag)**
  Calculates the predicted new response value for x in normalized space.
- **Real calc_nll ()**
  calculates the negative log likelihood function (based on covariance matrix)
- **void calc_grad_nll ()**
  Gets the gradient of the negative log likelihood function with respect to the correlation lengthscales, theta.
- **void get_grad_cov_vector ()**
  Calculate the derivatives of the covariance vector, with respect to each component of x.
- **void run_point_selection ()**
Runs the point selection algorithm, which will choose a subset of the training set with which to construct the GP model, and estimate the necessary parameters.

- void initialize_point_selection()
  
  Initializes the point selection routine by choosing a small initial subset of the training points.

- void pointsel_get_errors(RealArray &delta)
  
  Uses the current GP model to compute predictions at all of the training points and find the errors.

- int addpoint(int, IntArray &added_index)
  
  Adds a point to the effective training set. Returns 1 on success.

- int pointsel_addsel(const RealArray &delta)
  
  Accepts a vector of unsorted prediction errors, determines which points should be added to the effective training set, and adds them.

- Real maxval(const RealArray &)
  
  Returns the maximum value of the elements in a vector.

- void pointsel_write_points()
  
  Writes out the training set before and after point selection.

- void lhood_2d_grid_eval()
  
  For problems with 2D input, evaluates the negative log likelihood on a grid.

- void writex(const char[])
  
  Writes out the current training set (in original units) to a specified file.

- void writeCovMat(char[])
  
  Writes out the covariance matrix to a specified file.

### Static Private Member Functions

- static void negloglik(int mode, int n, const Teuchos::SerialDenseVector<int, double> &X, Real &fx, Teuchos::SerialDenseVector<int, double> &grad_x, int &result_mode)
  
  static function used by OPT++ as the objective function to optimize the hyperparameters in the covariance of the GP by minimizing the negative log likelihood

- static void constraint_eval(int mode, int n, const Teuchos::SerialDenseVector<int, double> &X, Teuchos::SerialDenseVector<int, double> &g, Teuchos::SerialDenseMatrix<int, double> &gradC, int &result_mode)
  
  static function used by OPT++ as the constraint function in the optimization of the negative log likelihood. Currently this function is empty: it is an unconstrained optimization.

- static double negloglikNCSU(const RealVector &x)
  
  function used by NCSUOptimizer to optimize negloglik objective

### Private Attributes

- Real approxValue
  
  value of the approximation returned by value()

- Real approxVariance
  
  value of the approximation returned by prediction_variance()

- RealMatrix trainPoints
  
  A 2-D array (num sample sites = rows, num vars = columns) used to create the Gaussian process.

- RealMatrix trainValues
A collection of response values; one response value per sample site.

- **RealVector** `trainMeans`  
  The mean of the input columns of `trainPoints`.

- **RealVector** `trainStdvs`  
  The standard deviation of the input columns of `trainPoints`.

- **RealMatrix** `normTrainPoints`  
  Current working set of normalized points upon which the GP is based.

- **RealMatrix** `trendFunction`  
  Matrix to hold the trend function.

- **RealMatrix** `betaCoeffs`  
  Matrix to hold the beta coefficients for the trend function.

- **RealSymMatrix** `covMatrix`  
  The covariance matrix where each element (i,j) is the covariance between points Xi and Xj in the initial set of samples.

- **RealMatrix** `covVector`  
  The covariance vector where each element (j,0) is the covariance between a new point X and point Xj from the initial set of samples.

- **RealMatrix** `approxPoint`  
  Point at which a prediction is requested. This is currently a single point, but it could be generalized to be a vector of points.

- **RealMatrix** `gradNegLogLikTheta`  
  Matrix to hold the gradient of the negative log likelihood with respect to the theta correlation terms.

- **Teuchos::SerialSpdDenseSolver**  
  The global solver for all computations involving the inverse of the covariance matrix.

- **RealMatrix** `gradCovVector`  
  A matrix, where each column is the derivative of the covVector with respect to a particular component of X.

- **RealMatrix** `normTrainPointsAll`  
  Set of all original samples available.

- **RealMatrix** `trainValuesAll`  
  All original samples available.

- **RealMatrix** `trendFunctionAll`  
  Trend function values corresponding to all original samples.

- **RealMatrix** `Rinv_YFB`  
  Matrix for storing inverse of correlation matrix $R^{-1}(Y-FB)$.

- **size_t** `numObs`  
  The number of observations on which the GP surface is built.

- **size_t** `numObsAll`  
  The original number of observations.

- **short** `trendOrder`  
  The number of variables in each X variable (number of dimensions of the problem).

- **RealVector** `thetaParams`
Theta is the vector of covariance parameters for the GP. We determine the values of theta by optimization. Currently, the covariance function is \( \theta[0] \ast \exp(-0.5 \ast \text{sume}) + \delta \ast \text{pow}(\sigma_g, 2) \). \text{sume} is the sum squared of weighted distances; it involves a sum of \( \theta[1] \ast (X_i(1) - X_j(1))^2 + \theta[2] \ast (X_i(2) - X_j(2))^2 + \ldots \) where \( X_i(1) \) is the first dimension value of multi-dimensional variable \( X \). \( \delta \ast \text{pow}(\sigma_g, 2) \) is a jitter term used to improve matrix computations. \( \delta \) is zero for the covariance between different points and 1 for the covariance between the same point. \( \sigma_g \) is the underlying process error.

- **Real procVar**
  The process variance, the multiplier of the correlation matrix.

- **IntArray pointsAddedIndex**
  Used by the point selection algorithm, this vector keeps track all points which have been added.

- **int cholFlag**
  A global indicator for success of the Cholesky factorization.

- **bool usePointSelection**
  A flag to indicate the use of point selection

### Static Private Attributes

- **static GaussProcApproximation * GPinstance**
  pointer to the active object instance used within the static evaluator

### Additional Inherited Members

#### 13.58.1 Detailed Description

Derived approximation class for Gaussian Process implementation.

The GaussProcApproximation class provides a global approximation (surrogate) based on a Gaussian process. The Gaussian process is built after normalizing the function values, with zero mean. Opt++ is used to determine the optimal values of the covariance parameters, those which minimize the negative log likelihood function.

#### 13.58.2 Constructor & Destructor Documentation

**GaussProcApproximation ( ) [inline]**

default constructor

alternate constructor used by EffGlobalOptimization and NonDGlobalReliability that does not use a problem database defaults here are no point selectinn and quadratic trend function.

#### 13.58.3 Member Function Documentation

**void GPmodel_apply ( const RealVector & new_x, bool variance_flag, bool gradients_flag ) [private]**

Function returns a response value using the GP surface.

The response value is computed at the design point specified by the RealVector function argument.

References Dakota::abort_handler(), GaussProcApproximation::approxPoint, GaussProcApproximation::get_cov_vector(), SharedApproxData::numVars, GaussProcApproximation::predict(), Approximation::sharedDataRep, GaussProcApproximation::trainMeans, and GaussProcApproximation::trainStdvs.

Referenced by GaussProcApproximation::gradient(), GaussProcApproximation::pointsel_get_errors(), GaussProcApproximation::prediction_variance(), and GaussProcApproximation::value().
13.58.4 Member Data Documentation

short trendOrder  [private]

The number of variables in each X variable (number of dimensions of the problem).

The order of the basis function for the mean of the GP If the order = 0, the trend is a constant, if the order = 1, trend is linear, if order = 2, trend is quadratic.

Referenced by GaussProcApproximation::GaussProcApproximation(), GaussProcApproximation::get_beta_coefficients(), GaussProcApproximation::get_trend(), GaussProcApproximation::GPmodel_build(), and GaussProcApproximation::predict().

The documentation for this class was generated from the following files:

- GaussProcApproximation.hpp
- GaussProcApproximation.cpp

13.59 GeneralReader Class Reference

Utility used in derived read_core to read in generic format.

Public Member Functions

- template<typename ArrayType >
  void operator() (std::istream &s, size_t start_index, size_t num_items, ArrayType &array_data, StringMultiArrayView label_array)

13.59.1 Detailed Description

Utility used in derived read_core to read in generic format.

The documentation for this class was generated from the following file:

- DakotaVariables.hpp

13.60 GeneralWriter Class Reference

Utility used in derived write_core to write in generic format.

Public Member Functions

- template<typename ArrayType >
  void operator() (std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array)

13.60.1 Detailed Description

Utility used in derived write_core to write in generic format.

The documentation for this class was generated from the following file:

- DakotaVariables.hpp
13.61  GetLongOpt Class Reference

GetLongOpt is a general command line utility from S. Manoharan (Advanced Computer Research Institute, Lyon, France).

Inheritance diagram for GetLongOpt:

```
GetLongOpt
    |    
   v    
CommandLineHandler
```

Public Types

- `enum OptType { Valueless, OptionalValue, MandatoryValue }

  enum for different types of values associated with command line options.

Public Member Functions

- `GetLongOpt (const char optmark= '-')`  
  Constructor.
- `~GetLongOpt ()`  
  Destructor.
- `int parse (int argc, char ∗ const argv)`  
  parse the command line args (argc, argv).
- `int parse (char ∗ const str, char ∗ const p)`  
  parse a string of options (typically given from the environment).
- `int enroll (const char ∗ const opt, const OptType t, const char ∗ const desc, const char ∗ const val)`  
  Add an option to the list of valid command options.
- `const char ∗ retrieve (const char ∗ const opt) const`  
  Retrieve value of option.
- `void usage (std::ostream &outfile=Cout) const`  
  Print usage information to outfile.
- `void usage (const char ∗ str)`  
  Change header of usage output to str.
- `void store (const char ∗ name, const char ∗ value)`  
  Store a specified option value.

Private Member Functions

- `char ∗ basename (char ∗ const p) const`  
  extract the base name from a string as delimited by ‘/’
- `int setcell (Cell ∗ c, char ∗ valtoken, char ∗ nexttoken, const char ∗ p)`  
  internal convenience function for setting Cell::value
Private Attributes

- Cell * table
  - option table
- const char * ustring
  - usage message
- char * pname
  - program basename
- char optmarker
  - option marker
- int enroll_done
  - finished enrolling
- Cell * last
  - last entry in option table

13.61.1 Detailed Description

GetLongOpt is a general command line utility from S. Manoharan (Advanced Computer Research Institute, Lyon, France).

GetLongOpt manages the definition and parsing of "long options." Command line options can be abbreviated as long as there is no ambiguity. If an option requires a value, the value should be separated from the option either by whitespace or an ":=".

13.61.2 Member Enumeration Documentation

enum OptType

enum for different types of values associated with command line options.

Enumerator

- Valueless  option that may never have a value
- OptionalValue  option with optional value
- MandatoryValue  option with required value

13.61.3 Constructor & Destructor Documentation

GetLongOpt ( const char optmark = ' ' )

Constructor.

Constructor for GetLongOpt takes an optional argument: the option marker. If unspecified, this defaults to ":", the standard (?) Unix option marker.

13.61. GETLONGOPT CLASS REFERENCE

13.61.4 Member Function Documentation

**int parse ( int argc, char *const argv )**

parse the command line args (argc, argv).

A return value < 1 represents a parse error. Appropriate error messages are printed when errors are seen. parse returns the the optind (see getopt(3)) if parsing is successful.


Referenced by CommandLineHandler::check_usage().

**int parse ( char *const str, char *const p )**

parse a string of options (typically given from the environment).

A return value < 1 represents a parse error. Appropriate error messages are printed when errors are seen.

parse takes two strings: the first one is the string to be parsed and the second one is a string to be prefixed to the parse errors.


**int enroll ( const char *const opt, const OptType t, const char *const desc, const char *const val )**

Add an option to the list of valid command options.

enroll adds option specifications to its internal database. The first argument is the option sting. The second is an enum saying if the option is a flag (Valueless), if it requires a mandatory value (MandatoryValue) or if it takes an optional value (OptionalValue). The third argument is a string giving a brief description of the option. This description will be used by GetLongOpt::usage. GetLongOpt, for usage-printing, uses \{val\} to represent values needed by the options. \{<$val>\} is a mandatory value and \{$val\}\} is an optional value. The final argument to enroll is the default string to be returned if the option is not specified. For flags (options with Valueless), use "" (empty string, or in fact any arbitrary string) for specifying TRUE and 0 (null pointer) to specify FALSE.

References GetLongOpt::enroll_done, GetLongOpt::last, and GetLongOpt::table.

Referenced by CommandLineHandler::initialize_options().

**const char * retrieve ( const char *const opt ) const**

Retrieve value of option.

The values of the options that are enrolled in the database can be retrieved using retrieve. This returns a string and this string should be converted to whatever type you want. See atoi, atof, atol, etc. If a "parse" is not done before retrieving all you will get are the default values you gave while enrolling! Ambiguities while retrieving (may happen when options are abbreviated) are resolved by taking the matching option that was enrolled last. For example, -$v will expand to -verify. If you try to retrieve something you didn’t enroll, you will get a warning message.

References GetLongOpt::optmarker, and GetLongOpt::table.

Referenced by CommandLineHandler::check_usage(), ProgramOptions::manage_run_modes(), ProgramOptions::ProgramOptions(), and CommandLineHandler::read_restart_evals().

**void usage ( const char * str ) [inline]**

Change header of usage output to str.

GetLongOpt::usage is overloaded. If passed a string "str", it sets the internal usage string to "str". Otherwise it simply prints the command usage.

References GetLongOpt::ustring.
The documentation for this class was generated from the following files:

- CommandLineHandler.hpp
- CommandLineHandler.cpp

### 13.62 Graphics Class Reference

The Graphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics; there is only one instance of this OutputManager::dakotaGraphics.

#### Public Member Functions

- **Graphics ()**
  - constructor
- **~Graphics ()**
  - destructor
- **void create_plots_2d (const Variables &vars, const Response &response)**
  - creates the 2d graphics window and initializes the plots
- **void add_datapoint (int graphics_cntr, const Variables &vars, const Response &response)**
  - adds data to each window in the 2d graphics based on the results of a model evaluation
- **void add_datapoint (int i, double x, double y)**
  - adds data to a single window in the 2d graphics
- **void new_dataset (int i)**
  - creates a separate line graphic for subsequent data points for a single window in the 2d graphics
- **void close ()**
  - close graphics windows
- **void set_x_labels2d (const char *x_label)**
  - set x label for each plot equal to x_label
- **void set_y_labels2d (const char *y_label)**
  - set y label for each plot equal to y_label
- **void set_x_label2d (int i, const char *x_label)**
  - set x label for ith plot equal to x_label
- **void set_y_label2d (int i, const char *y_label)**
  - set y label for ith plot equal to y_label

#### Private Attributes

- **Graphics2D * graphics2D**
  - pointer to the 2D graphics object
- **bool win2dOn**
  - flag to indicate if 2D graphics window is active

### 13.62.1 Detailed Description

The Graphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics; there is only one instance of this OutputManager::dakotaGraphics.
13.62.2 Member Function Documentation

```c
void create_plots_2d ( const Variables & vars, const Response & response )
```

creates the 2d graphics window and initializes the plots.

Sets up a single event loop for duration of the dakotaGraphics object, continuously adding data to a single
window. There is no reset. To start over with a new data set, you need a new object (delete old and instantiate
new).

References Variables::continuous_variable_labels(), Variables::cv(), Variables::discrete_int_variable_labels(),
Variables::discrete_real_variable_labels(), Variables::div(), Variables::drv(), Response::function_labels(), Graphics-
::graphics2D, Response::num_functions(), Dakota::re_match(), and Graphics::win2dOn.

Referenced by SurrBasedMinimizer::initialize_graphics(), NonDReliability::initialize_graphics(), and Iterator-
::initialize_graphics().

```c
void add_datapoint ( int graphics_cntr, const Variables & vars, const Response & response )
```

adds data to each window in the 2d graphics based on the results of a model evaluation.

Adds data to each 2d plot and each tabular data column (one for each active variable and for each response
function). graphicsCntr is used for the x axis in the graphics and the first column in the tabular data.

References Response::active_set_request_vector(), Variables::continuous_variables(), Variables::discrete_int-
variables(), Variables::discrete_real_variables(), Response::function_values(), Graphics::graphics2D, and Graphics-
::win2dOn.

Referenced by OutputManager::add_datapoint(), NonDLocalReliability::mean_value(), and NonDLocalReliability-
::update_level_data().

```c
void add_datapoint ( int i, double x, double y )
```

adds data to a single window in the 2d graphics.

Adds data to a single 2d plot. Allows complete flexibility in defining other kinds of x-y plotting in the 2D
graphics.

References Graphics::graphics2D, and Graphics::win2dOn.

```c
void new_dataset ( int i )
```

creates a separate line graphic for subsequent data points for a single window in the 2d graphics.

Used for displaying multiple data sets within the same plot.

References Graphics::graphics2D, and Graphics::win2dOn.

Referenced by NonDLocalReliability::update_level_data().

The documentation for this class was generated from the following files:

- DakotaGraphics.hpp
- DakotaGraphics.cpp

13.63 GridApplicInterface Class Reference

Derived application interface class which spawns simulation codes using grid services such as Condor or Globus.

Inheritance diagram for GridApplicInterface:
### Public Member Functions

- **GridApplicInterface** (const ProblemDescDB &problem_db)
  
  _constructor_

- **~GridApplicInterface** ()
  
  _destructor_

- **void derived_map** (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)
  
  Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.

- **void derived_map_asynch** (const ParamResponsePair &pair)
  
  Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.

- **void wait_local_evaluations** (PRPQueue &prp_queue)
  
  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.

- **void test_local_evaluations** (PRPQueue &prp_queue)
  
  Convenience function for common code between wait and noWait case.

- **int synchronous_local_analysis** (int analysis_id)

### Protected Member Functions

- **bool grid_file_test** (const String &root_file)
  
  test file(s) for existence based on root_file name

### Protected Attributes

- **IntSet idSet**
  
  Set of function evaluation id’s for active asynchronous system call evaluations.

- **IntShortMap failCountMap**
  
  map linking function evaluation id’s to number of response read failures

- **start_grid_computing_t start_grid_computing**
  
  handle to dynamically linked start_grid_computing function

- **perform_analysis_t perform_analysis**
13.63.1 Detailed Description

Derived application interface class which spawns simulation codes using grid services such as Condor or Globus. This class is currently a modified copy of SysCallApplicInterface adapted for use with an external grid services library which was dynamically linked using dlopen() services.

13.63.2 Member Function Documentation

int synchronous_local_analysis ( int analysis_id ) [inline], [virtual]

This code provides the derived function used by ApplicationInterface::serve_analyses_synch(). TODO - allow local analyses?????

Reimplemented from ApplicationInterface.

References SysCallApplicInterface::spawn_analysis_to_shell().

The documentation for this class was generated from the following files:

• GridApplicInterface.hpp
• GridApplicInterface.cpp

13.64 HierarchSurrBasedLocalMinimizer Class Reference

Class for multilevel-multifidelity optimization algorithm.

Inheritance diagram for HierarchSurrBasedLocalMinimizer:

```
+-----------------+                      +-----------------+
|                 |                      |                 |
|  Iterator       |                      |  HierarchSurrBasedLocalMinimizer |
|                 |                      |                 |
|                +-----------------+                      +-----------------+
|                |  Minimizer           |                      |  SurrBasedMinimizer               |
|                +-----------------+                      +-----------------+
|                |                        |                      |  SurrBasedLocalMinimizer          |
|                +-----------------+                      +-----------------+
```

**Public Member Functions**

- HierarchSurrBasedLocalMinimizer (ProblemDescDB &problem_db, Model &model)
  
  *constructor*

- ~HierarchSurrBasedLocalMinimizer ()

  *destructor*
Protected Member Functions

- **void pre_run ()**
  
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- **void post_run (std::ostream &s)**
  
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
- **SurrBasedLevelData & trust_region ()**
  
  return the active SurrBasedLevelData instance
- **void update_trust_region ()**
  
  update the trust region bounds, strictly contained within global bounds
- **void build ()**
- **void minimize ()**
- **void verify ()**
  
  verify the approximate iterate and update the trust region for the next approximate optimization cycle
- **unsigned short converged ()**
  
  return the convergence code for the truth level of the trust region hierarchy

Private Member Functions

- **void build_center_truth (size_t tr_index)**
  
  build the hierarchical approximation for a particular level by computing center truth within the HierarchSurrModel
- **void find_center_truth (size_t tr_index, bool search_db=false)**
  
  Retrieve or evaluate SurrBasedLevelData::responseCenterTruthUncorrected.
- **void find_center_approx (size_t tr_index)**
  
  Retrieve or evaluate SurrBasedLevelData::responseCenterApproxUncorrected.
- **void find_star_truth (size_t tr_index, bool search_db=false)**
  
  Retrieve or evaluate SurrBasedLevelData::responseStarTruthUncorrected.
- **void find_star_approx (size_t tr_index)**
  
  Retrieve or evaluate SurrBasedLevelData::responseStarApproxUncorrected.
- **void correct_center_truth (size_t tr_index)**
  
  apply recursive corrections to SurrBasedLevelData:: responseCenterTruthUncorrected and store in SurrBasedLevelData:: responseCenterTruthCorrected
- **void correct_center_approx (size_t tr_index)**
  
  apply recursive corrections to SurrBasedLevelData:: responseCenterApproxUncorrected and store in SurrBasedLevelData:: responseCenterApproxCorrected
- **void correct_star_truth (size_t tr_index)**
  
  apply recursive corrections to SurrBasedLevelData:: responseStarTruthUncorrected and store in SurrBasedLevelData:: responseStarTruthCorrected
- **void correct_star_approx (size_t tr_index)**
  
  apply recursive corrections to SurrBasedLevelData:: responseStarApproxUncorrected and store in SurrBasedLevelData:: responseStarApproxCorrected
- **void set_model_states (size_t tr_index)**
  
  activate model forms and, optionally, discretization levels within the HierarchSurrModel associated with trust-Regions[tr_index]
13.64. HIERARCHSURRBASEDLOCALMINIMIZER CLASS REFERENCE

- void update_trust_region (size_t tr_index_start)
  
  update trust region bounds, recurring top-down from tr_index_start
- void verify (size_t tr_index)
  
  Verify approximate step with truth model for trust region level tr_index.
- RealVector multigrid_recursion (const RealVector &xk, int k)
- void multigrid_driver (const Variables &x0)
- RealVector optimize (const RealVector &x, int max_iter, int index)
- RealVector linesearch (const RealVector &xk, const RealVector &pk, double alpha0)

Private Attributes

- size_t numFid
  
  number of ordered model fidelities within iteratedModel (a HierarchSurrModel)
- SizetArray numLev
  
  number of discretization levels per ordered model fidelity
- bool multiLev
  
  flag indicating presence of more than one level per fidelity
- size_t minimizeIndex
  
  index for trustRegions at which the minimization is performed
- std::vector<SurrBasedLevelData> trustRegions
- bool nestedTrustRegions

Additional Inherited Members

13.64.1 Detailed Description

Class for multilevel-multifidelity optimization algorithm.

This minimizer uses SurrogateModel(s) to perform minimization leveraging multiple model forms and discretization levels.

13.64.2 Member Function Documentation

void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

  pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s pre_run(), if implemented, typically before performing its own implementation steps.

Reimplemented from Iterator.

References SurrBasedLocalMinimizer::approxSetRequest, Model::current_variables(), Iterator::iteratedModel, HierarchySurrBasedLocalMinimizer::numFid, SurrBasedLocalMinimizer::origTrustRegionFactor, SurrBasedLocalMinimizer::pre_run(), and SurrBasedLocalMinimizer::truthSetRequest.
void post_run ( std::ostream & s ) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s post_run(), typically after performing its own implementation steps.

Reimplemented from Minimizer.

References SurrBasedLocalMinimizer::approxSubProbModel, Iterator::bestResponseArray, Iterator::bestVariablesArray, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), SurrBasedLocalMinimizer::globalLowerBnds, SurrBasedLocalMinimizer::globalUpperBnds, and SurrBasedLocalMinimizer::post_run().

void build ( ) [protected], [virtual]

Step 2 in SurrBasedLocalMinimizer::core_run().

Implements SurrBasedLocalMinimizer.

References Dakota::NPOS, HierarchSurrBasedLocalMinimizer::build_center_truth(), DiscrepancyCorrection::compute(), HierarchSurrBasedLocalMinimizer::correct_center_approx(), HierarchSurrBasedLocalMinimizer::correct_center_truth(), HierarchSurrBasedLocalMinimizer::correct_star_approx(), Model::discrepancy_correction(), HierarchSurrBasedLocalMinimizer::find_center_approx(), SurrBasedLocalMinimizer::globalLowerBnds, SurrBasedLocalMinimizer::globalUpperBnds, SurrBasedLocalMinimizer::hard_convergence_check(), Iterator::iteratedModel, SurrBasedLocalMinimizer::minimizeCycles, HierarchSurrBasedLocalMinimizer::minimizeIndex, SurrBasedLocalMinimizer::origTrustRegionFactor, SurrBasedLocalMinimizer::print_convergence_code(), SurrBasedLocalMinimizer::reset_multipliers(), SurrBasedLocalMinimizer::reset_penalties(), HierarchSurrBasedLocalMinimizer::set_model_states(), HierarchSurrBasedLocalMinimizer::update_trust_region(), and HierarchSurrBasedLocalMinimizer::verify().

void minimize ( ) [protected], [virtual]

Step 3 in SurrBasedLocalMinimizer::core_run().

Reimplemented from SurrBasedLocalMinimizer.

References SurrBasedMinimizer::approxSubProbMinimizer, HierarchSurrBasedLocalMinimizer::find_star_approx(), Iterator::iteratedModel, SurrBasedLocalMinimizer::minimize(), HierarchSurrBasedLocalMinimizer::minimizeIndex, Model::model_rep(), SurrBasedLocalMinimizer::recastSubProb, Model::recursive_apply(), Iterator::response_results(), HierarchSurrBasedLocalMinimizer::set_model_states(), SurrBasedLocalMinimizer::update_approx_sub_problem(), and Iterator::variables_results().

void update_trust_region ( size_t tr_index_start ) [private]

update trust region bounds, recurring top-down from tr_index_start

Step 1 in SurrBasedLocalMinimizer::core_run().

References Dakota::abort_handler(), SurrBasedLocalMinimizer::globalLowerBnds, SurrBasedLocalMinimizer::globalUpperBnds, HierarchSurrBasedLocalMinimizer::minimizeIndex, Minimizer::numContinuousVars, and SurrBasedLocalMinimizer::update_trust_region_data().

void verify ( size_t tr_index ) [private]

Verify approximate step with truth model for trust region level tr_index.

Step 4 in SurrBasedLocalMinimizer::core_run().
13.65  HierarchSurrModel Class Reference

Derived model class within the surrogate model branch for managing hierarchical surrogates (models of varying fidelity).

Inheritance diagram for HierarchSurrModel:

```
Model
   |
   v
SurrogateModel
   |
   v
HierarchSurrModel
```

### Public Member Functions

- **HierarchSurrModel (ProblemDescDB &problem_db)**
  
  constructor

- **~HierarchSurrModel ()**
  
  destructor

- **DiscrepancyCorrection & discrepancy_correction ()**
  
  return the active DiscrepancyCorrection instance

- const unsigned short **correction_mode ()** const

- void **correction_mode** (unsigned short corr_mode)

### Protected Member Functions

- bool **initialize_mapping** (ParLevLIter pl_iter)
  
  Perform any global updates prior to individual evaluate() calls.

- bool **finalize_mapping ()**
  
  restore state in preparation for next initialization

- void **derived_evaluate** (const ActiveSet &set)
  
  portion of evaluate() specific to HierarchSurrModel

- void **derived_evaluate_nowait** (const ActiveSet &set)
  
  portion of evaluate_nowait() specific to HierarchSurrModel

- const IntResponseMap & **derived_synchronize ()**
portion of synchronize() specific to HierarchSurrModel

- const IntResponseMap & derived_synchronize_nowait()

portion of synchronize_nowait() specific to HierarchSurrModel

- Model & surrogate_model()
  return the active low fidelity model

- void surrogate_model_indices(size_t lf_model_index, size_t lf_soln_lev_index=NPOS)
  set the indices identifying the active low fidelity model

- void surrogate_model_indices(const SizetSizetPair &lf_form_level)
  set the index pair identifying the active low fidelity model

- const SizetSizetPair & surrogate_model_indices() const
  return the indices identifying the active low fidelity model

- SizetSizet2DPair get_indices()
  return pair of active low fidelity and high fidelity model indices

- Model & truth_model()
  return the active high fidelity model

- void truth_model_indices(size_t hf_model_index, size_t hf_soln_lev_index=NPOS)
  set the indices identifying the active high fidelity model

- void truth_model_indices(const SizetSizetPair &hf_form_level)
  set the index pair identifying the active high fidelity model

- const SizetSizetPair & truth_model_indices() const
  return the indices identifying the active high fidelity model

- void derived_subordinate_models(ModelList &ml, bool recurse_flag)
  return orderedModels and, optionally, their sub-model recursions

- void primary_response_fn_weights(const RealVector &wts, bool recurse_flag=true)
  set the relative weightings for multiple objective functions or least squares terms and optionally recurses into LF/HF models

- void surrogate_response_mode(short mode)
  set responseMode and pass any bypass request on to the high fidelity model for any lower-level surrogate recursions

- void surrogate_function_indices(const IntSet &surr_fn_indices)
  (re)set the surrogate index set in SurrogateModel::surrogateFnIndices

- void build_approximation()
  use the high fidelity model to compute the truth values needed for correction of the low fidelity model results

- void component_parallel_mode(short mode)
  update component parallel mode for supporting parallelism in the low ad high fidelity models

- InIntPair estimate_partition_bounds(int max_eval_concurrency)
  estimate the minimum and maximum partition sizes that can be utilized by this Model

- void derived_init_communicators(ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  set up parallel operations for the array of ordered model fidelities

- void derived_init_serial()
  set up serial operations for the array of ordered model fidelities

- void derived_set_communicators(ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  set active parallel configuration within the current low and high fidelity models identified by {low,high}Fidelity-Indices
• void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  deallocate communicator partitions for the HierarchSurrModel (request forwarded to the array of ordered model fidelities)
• void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)
  Service the low and high fidelity model job requests received from the master; completes when termination message received from stop_servers().
• void stop_servers ()
  Executed by the master to terminate the low and high fidelity model server operations when iteration on the HierarchSurrModel is complete.
• void inactive_view (short view, bool recurse_flag=true)
  update the Model’s inactive view based on higher level (nested) context and optionally recurse into
• void set_evaluation_reference ()
  set the evaluation counter reference points for the HierarchSurrModel (request forwarded to the low and high fidelity models)
• void fine_grained_evaluation_counters ()
  request fine-grained evaluation reporting within the low and high fidelity models
• void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const
  print the evaluation summary for the HierarchSurrModel (request forwarded to the low and high fidelity models)
• void warm_start_flag (const bool flag)
  set the warm start flag, including the orderedModels

Private Member Functions
• void check_interface_instance ()
  update sameInterfaceInstance based on interface ids for models identified by current {low,high}FidelityIndices
• void update_model (Model &model)
  update the passed model (one of the ordered models) with data that could change per function evaluation (active variable values/bounds)
• void init_model (Model &model)
  update the passed model (one of the ordered models) with data that could change once per set of evaluations (e.g., an outer iterator execution), including active variable labels, inactive variable values/bounds/labels, and linear/nonlinear constraint coeffs/bounds
• void derived_synchronize_sequential (IntResponseMap &hf_resp_map_rekey, IntResponseMap &lf_resp_map_rekey, bool block)
  called from derived_synchronize() and derived_synchronize_nowait() to extract and rekey response maps using blocking or nonblocking synchronization on the LF and HF models
• void derived_synchronize_competing ()
  called from derived_synchronize() for case of distinct models/interfaces with competing LF/HF job queues
• void derived_synchronize_combine (const IntResponseMap &hf_resp_map, IntResponseMap &lf_resp_map, IntResponseMap &combined_resp_map)
  combine the HF and LF response maps into a combined response map
• void derived_synchronize_combine_nowait (const IntResponseMap &hf_resp_map, IntResponseMap &lf_resp_map, IntResponseMap &combined_resp_map)
  combine the available components from HF and LF response maps into a combined response map
• void resize_response ()
CHAPTER 13. CLASS DOCUMENTATION

```
resize currentResponse based on responseMode
• void compute_apply_delta (IntResponseMap &lf_resp_map)
  helper function used in the AUTO_CORRECTED_SURROGATE responseMode for computing a correction and
  applying it to lf_resp_map
• void single_apply (const Variables &vars, Response &resp, const SizetSizet2DPair &indices)
  helper function for applying a single deltaCorr correction corresponding to indices
• void recursive_apply (const Variables &vars, Response &resp)
  helper function for applying a correction across a sequence of model forms or discretization levels
• void stop_model (size_t ordered_model_index)
  stop the servers for the orderedModels instance identified by the passed index

Private Attributes
• DiscrepCorrMap deltaCorr
  manages construction and application of correction functions that are applied to a surrogate model (DataFitSurr
  or HierarchSurr) in order to reproduce high fidelity data.
• short corrOrder
  order of correction: 0, 1, or 2
• unsigned short correctionMode
• std::vector<SizetSizet2DPair> corrSequence
  vector to specify a sequence of discrepancy corrections to apply in AUTO_CORRECTED_SURROGATE mode
• ModelArray orderedModels
  Ordered sequence (low to high) of model fidelities. Models are of arbitrary type and supports recursions.
• SizetSizetPair lowFidelityIndices
  index of the low fidelity model that is currently active within orderedModels; provides approximate low fidelity
  function evaluations.
• SizetSizetPair highFidelityIndices
  index of the high fidelity model that is currently active within orderedModels; provides truth evaluations for com-
  puting corrections to the low fidelity results.
• bool sameModelInstance
  flag indicating that the {low,high}FidelityIndices correspond to the same model instance, requiring modifications
  to updating and evaluation scheduling processes
• bool sameInterfaceInstance
  flag indicating that the models identified by {low,high}FidelityIndices employ the same interface instance, requiring
  modifications to evaluation scheduling processes
• SizetSizetPair componentParallelIndices
  store index pair that is active in component_parallel_mode()
• std::map<SizetSizetPair, Response> truthResponseRef
  map of reference truth (high fidelity) responses computed in build_approximation() and used for calculating correc-
  tions
• IntResponseMap cachedTruthRespMap
  map of truth (high-fidelity) responses retrieved in derived_synchronize_nowait() that could not be returned since
  corresponding low-fidelity response portions were still pending
```
Additional Inherited Members

13.65.1 Detailed Description

Derived model class within the surrogate model branch for managing hierarchical surrogates (models of varying fidelity).

The HierarchSurrModel class manages hierarchical models of varying fidelity. The class contains an ordered array of model forms (fidelity ordered from low to high), where each model form may also contain a set of solution levels (space/time discretization, convergence tolerances, etc.). At run time, one of these combinations is activated as the low fidelity model and used to perform approximate function evaluations, while another of these combinations is activated as the high fidelity model and used to provide truth evaluations for computing corrections to the low fidelity results.

13.65.2 Member Function Documentation

bool initialize_mapping ( ParLevLIter pl_iter ) [protected], [virtual]

Perform any global updates prior to individual evaluate() calls.

Inactive variables must be propagated when a HierarchSurrModel is employed by a sub-iterator (e.g., OUU with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::initialize_mapping().

Reimplemented from Model.
References HierarchSurrModel::init_model(), SurrogateModel::initialize_mapping(), and HierarchSurrModel::orderedModels.

bool finalize_mapping ( ) [protected], [virtual]

restore state in preparation for next initialization

Inactive variables must be propagated when a HierarchSurrModel is employed by a sub-iterator (e.g., OUU with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::initialize_mapping().

Reimplemented from Model.
References SurrogateModel::finalize_mapping(), and HierarchSurrModel::orderedModels.

void derived_evaluate ( const ActiveSet & set ) [protected], [virtual]

portion of evaluate() specific to HierarchSurrModel

Compute the response synchronously using LF model, HF model, or both (mixed case). For the LF model portion, compute the high fidelity response if needed with build_approximation(), and, if correction is active, correct the low fidelity results.

Reimplemented from Model.
References Response::active_set(), SurrogateModel::aggregate_response(), SurrogateModel::approxBuilds, SurrogateModel::asv_mapping(), HierarchSurrModel::build_approximation(), HierarchSurrModel::component_parallel_mode(), Response::copy(), Model::current_response(), Model::currentResponse, Model::currentVariables, HierarchSurrModel::deltaCorr, Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate(), SurrogateModel::force_rebuild(), HierarchSurrModel::get_indices(), Model::highFidelityIndices, HierarchSurrModel::lowFidelityIndices, HierarchSurrModel::orderedModels, Model::outputLevel, HierarchSurrModel::recursive_apply(), ActiveSet::request_vector(), SurrogateModel::response_mapping(), SurrogateModel::responseMode, HierarchSurrModel::sameModelInstance, Model::solution_level_index(), SurrogateModel::surrModelEvalCntr, Response::update(), and HierarchSurrModel::update_model().
void derived_evaluate_nowait ( const ActiveSet & set ) [protected], [virtual]

portion of evaluate_nowait() specific to HierarchSurrModel

Compute the response asynchronously using LF model, HF model, or both (mixed case). For the LF model portion, compute the high fidelity response with build_approximation() (for correcting the low fidelity results in derived_synchronize() and derived_synchronize_nowait()) if not performed previously.

Reimplemented from Model.

References SurrogateModel::approxBuilds, SurrogateModel::asv_mapping(), Model::async_flag(), HierarchSurrModel::build_approximation(), SurrogateModel::cachedApproxRespMap, HierarchSurrModel::cachedTruthRespMap, HierarchSurrModel::component_parallel_mode(), Response::copy(), Variables::copy(), Model::current_response(), Model::currentVariables, ActiveSet::derivative_vector(), Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), SurrogateModel::force_rebuild(), Model::hierarchicalTagging, HierarchSurrModel::highFidelityIndices, HierarchSurrModel::lowFidelityIndices, HierarchSurrModel::orderedModels, SurrogateModel::rawVarsMap, HierarchSurrModel::recursive_apply(), ActiveSet::request_vector(), SurrogateModel::responseMode, HierarchSurrModel::sameModelInstance, Model::solution_level_index(), SurrogateModel::surrIdMap, SurrogateModel::surrModelEvalCntr, SurrogateModel::truthIdMap, and HierarchSurrModel::update_model.

const IntResponseMap & derived_synchronize ( ) [protected], [virtual]

portion of synchronize() specific to HierarchSurrModel

Blocking retrieval of asynchronous evaluations from LF model, HF model, or both (mixed case). For the LF model portion, apply correction (if active) to each response in the array. derived_synchronize() is designed for the general case where derived_evaluate_nowait() may be inconsistent in its use of low fidelity evaluations, high fidelity evaluations, or both.

Reimplemented from Model.

References HierarchSurrModel::derived_synchronize_combine(), HierarchSurrModel::derived_synchronize_combine(), HierarchSurrModel::derived_synchronize_competing(), HierarchSurrModel::derived_synchronize_competing(), HierarchSurrModel::derived_synchronize_competing(), HierarchSurrModel::sameInterfaceInstance, HierarchSurrModel::sameModelInstance, SurrogateModel::surrIdMap, SurrogateModel::surrResponseMap, and SurrogateModel::truthIdMap.

const IntResponseMap & derived_synchronize_nowait ( ) [protected], [virtual]

portion of synchronize_nowait() specific to HierarchSurrModel

Nonblocking retrieval of asynchronous evaluations from LF model, HF model, or both (mixed case). For the LF model portion, apply correction (if active) to each response in the map. derived_synchronize_nowait() is designed for the general case where derived_evaluate_nowait() may be inconsistent in its use of actual evals, approx evals, or both.

Reimplemented from Model.

References HierarchSurrModel::derived_synchronize_combine_nowait(), HierarchSurrModel::derived_synchronize_competing(), and SurrogateModel::surrResponseMap.

Referenced by HierarchSurrModel::derived_synchronize_competing().

The documentation for this class was generated from the following files:

- HierarchSurrModel.hpp
- HierarchSurrModel.cpp

13.66 Interface Class Reference

Base class for the interface class hierarchy.
Inheritance diagram for Interface:

```
<table>
<thead>
<tr>
<th>Interface</th>
</tr>
</thead>
<tbody>
<tr>
<td>ApplicationInterface</td>
</tr>
<tr>
<td>ApproximationInterface</td>
</tr>
<tr>
<td>DirectApplicInterface</td>
</tr>
<tr>
<td>ProcessApplicInterface</td>
</tr>
<tr>
<td>MatlabInterface</td>
</tr>
<tr>
<td>PythonInterface</td>
</tr>
<tr>
<td>ScilabInterface</td>
</tr>
<tr>
<td>TestDriverInterface</td>
</tr>
<tr>
<td>ParallelDirectApplicInterface</td>
</tr>
<tr>
<td>SerialDirectApplicInterface</td>
</tr>
</tbody>
</table>
```

**Public Member Functions**

- **Interface ()**  
  *default constructor*
- **Interface (ProblemDescDB &problem_db)**  
  *standard constructor for envelope*
- **Interface (const Interface &interface_in)**  
  *copy constructor*
- **virtual ~Interface ()**  
  *destructor*
- **Interface operator= (const Interface &interface_in)**  
  *assignment operator*
- **virtual void map (const Variables &vars, const ActiveSet &set, Response &response, bool asynch_flag=false)**  
  *the function evaluator: provides a "mapping" from the variables to the responses.*
- **virtual const IntResponseMap & synchronize ()**  
  *reverses data from a series of asynchronous evaluations (blocking)*
- **virtual const IntResponseMap & synchronize_nowait ()**  
  *reverses data from a series of asynchronous evaluations (nonblocking)*
- **virtual void serve_evaluations ()**  
  *evaluation server function for multiprocessor executions*
- **virtual void stop_evaluation_servers ()**  
  *send messages from iterator rank 0 to terminate evaluation servers*
- **virtual void init_communicators (const IntArray &message_lengths, int max_eval_concurrency)**  
  *allocate communicator partitions for concurrent evaluations within an iterator and concurrent multiprocessor analyses within an evaluation.*
- **virtual void set_communicators (const IntArray &message_lengths, int max_eval_concurrency)**
set the local parallel partition data for an interface (the partitions are already allocated in ParallelLibrary).

- virtual void init_serial()
  reset certain defaults for serial interface objects.
- virtual int async_local_evaluation_concurrency() const
  return the user-specified concurrency for async local evaluations
- virtual short interface_synchronization() const
  return the user-specified interface synchronization
- virtual int minimum_points(bool constraint_flag) const
  returns the minimum number of points required to build a particular ApproximationInterface (used by DataFitSurrModels).
- virtual int recommended_points(bool constraint_flag) const
  returns the recommended number of points required to build a particular ApproximationInterface (used by DataFitSurrModels).
- virtual void approximation_function_indices(const IntSet &approx_fn_indices)
  set the (currently active) approximation function index set
- virtual void update_approximation(const Variables &vars, const IntResponsePair &response_pr)
  updates the anchor point for an approximation
- virtual void update_approximation(const RealMatrix &samples, const IntResponseMap &resp_map)
  updates the current data points for an approximation
- virtual void update_approximation(const VariablesArray &vars_array, const IntResponseMap &resp_map)
  updates the current data points for an approximation
- virtual void append_approximation(const Variables &vars, const IntResponsePair &response_pr)
  appends a single point to an existing approximation
- virtual void append_approximation(const RealMatrix &samples, const IntResponseMap &resp_map)
  appends multiple points to an existing approximation
- virtual void append_approximation(const VariablesArray &vars_array, const IntResponseMap &resp_map)
  appends multiple points to an existing approximation
- virtual void build_approximation(const RealVector &cl_bnds, const RealVector &cu_bnds, const IntVector &dl_bnds, const IntVector &du_bnds, const RealVector &dlbnds, const RealVector &dubnds)
  builds the approximation
- virtual void export_approximation()
  export the approximation to disk
- virtual void rebuild_approximation(const BoolDeque &rebuild_deque)
  rebuilds the approximation after a data update
- virtual void pop_approximation(bool save_surr_data)
  removes data from last append from the approximation
- virtual void push_approximation()
  retrieves approximation data from a previous state (negates pop)
- virtual bool push_available()
  queries the approximation for the ability to retrieve a previous increment
- virtual void finalize_approximation()
  finalizes the approximation by applying all trial increments
- virtual void store_approximation(size_t index=NPOS)
move the current approximation into storage for later combination; the index of the stored approximation can be
passed to allow replacement instead of augmentation (default is push_back)
• virtual void restore_approximation (size_t index=NPOS)
  return an approximation from storage; the index identifies a particular stored data set (default is pop_back from stored)
• virtual void remove_stored_approximation (size_t index=NPOS)
  remove a stored approximation, due to redundancy with the current approximation, prior to combination (default for no index is pop_back)
• virtual void combine_approximation (short corr_type)
  combine the current approximation with previously stored data sets
• virtual Real2DArray cv_diagnostics (const StringArray &metric_types, unsigned num_folds)
  approximation cross-validation quality metrics per response function
• virtual RealArray challenge_diagnostics (const String &metric_type, const RealMatrix &challenge_pts)
  approximation challenge data metrics per response function
• virtual void clear_current ()
  clears current data from an approximation interface
• virtual void clear_all ()
  clears all data from an approximation interface
• virtual void clear_popped ()
  clears bookkeeping for popped data sets from an approximation interface
• virtual SharedApproxData & shared_approximation ()
  retrieve the SharedApproxData within an ApproximationInterface
• virtual std::vector<Approximation> & approximations ()
  retrieve the Approximations within an ApproximationInterface
• virtual const Pecos::SurrogateData & approximation_data (size_t index)
  retrieve the approximation data from a particular Approximation within an ApproximationInterface
• virtual const RealVectorArray & approximation_coefficients (bool normalized=false)
  retrieve the approximation coefficients from each Approximation within an ApproximationInterface
• virtual void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)
  set the approximation coefficients within each Approximation within an ApproximationInterface
• virtual const RealVector & approximation_variances (const Variables &vars)
  retrieve the approximation variances from each Approximation within an ApproximationInterface
• virtual const StringArray & analysis_drivers () const
  retrieve the analysis drivers specification for application interfaces
• virtual bool evaluation_cache () const
  return flag indicating usage of the global evaluation cache
• virtual bool restart_file () const
  return flag indicating usage of the restart file
• virtual void file_cleanup () const
  clean up any interface parameter/response files when aborting
• void cache_unmatched_response (int raw_id)
  migrate an unmatched response record from rawResponseMap to cachedResponseMap
void assign_rep (Interface *interface_rep, bool ref_count_incr=true)
  assign letter or replace existing letter with a new one

unsigned short interface_type () const
  returns the interface type

const String & interface_id () const
  returns the interface identifier

int evaluation_id () const
  returns the value of the (total) evaluation id counter for the interface

void fine_grained_evaluation_counters (size_t num_fns)
  set fineGrainEvalCounters to true and initialize counters if needed

void init_evaluation_counters (size_t num_fns)
  initialize fine grained evaluation counters, sizing if needed

void set_evaluation_reference ()
  set evaluation count reference points for the interface

void print_evaluation_summary (std::ostream &s, bool minimal_header, bool relative_count) const
  print an evaluation summary for the interface

bool multi_proc_eval () const
  returns a flag signaling the use of multiprocessor evaluation partitions

bool iterator_eval_dedicated_master () const
  returns a flag signaling the use of a dedicated master processor at the iterator-evaluation scheduling level

bool is_null () const
  function to check interfaceRep (does this envelope contain a letter?)

void eval_tag_prefix (const String &eval_id_str, bool append_iface_id=true)
  set the evaluation tag prefix (does not recurse)

Protected Member Functions

Interface (BaseConstructor, const ProblemDescDB &problem_db)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

Interface (NoDBBaseConstructor, size_t num_fns, short output_level)
  constructor initializes the base class part of letter classes (NoDBBaseConstructor used for on the fly instantiations without a DB)

void init_algebraic_mappings (const Variables &vars, const Response &response)
  Define algebraicACVIndices, algebraicACVIds, and algebraicFnIndices.

void asv_mapping (const ActiveSet &total_set, ActiveSet &algebraic_set, ActiveSet &core_set)
  define the evaluation requirements for algebraic_mappings() (algebraic_set) and the core Application/Approximation mapping (core_set) from the total Interface evaluation requirements (total_set)

void asv_mapping (const ActiveSet &algebraic_set, ActiveSet &total_set)
  map an algebraic ASV back to original total ordering for async recovery

void algebraic_mappings (const Variables &vars, const ActiveSet &algebraic_set, Response &algebraic_response)
  evaluate the algebraic_response using the AMPL solver library and the data extracted from the algebraic_mappings file
• void response_mapping (const Response &algebraic_response, const Response &core_response, Response &total_response)
  combine the response from algebraic_mappings() with the response from derived_map() to create the total response

• String final_eval_id_tag (int fn_eval_id)
  form and return the final evaluation ID tag, appending iface ID if needed

Protected Attributes

• unsigned short interfaceType
  the interface type: enum for system, fork, direct, grid, or approximation

• String interfaceId
  the interface specification identifier string from the DAKOTA input file

• bool algebraicMappings
  flag for the presence of algebraic_mappings that define the subset of an Interface’s parameter to response mapping that is explicit and algebraic.

• bool coreMappings
  flag for the presence of non-algebraic mappings that define the core of an Interface’s parameter to response mapping (using analysis_drivers for ApplicationInterface or functionSurfaces for ApproximationInterface).

• short outputLevel
  output verbosity level: {SILENT, QUIET, NORMAL, VERBOSE, DEBUG}_OUTPUT

• int currEvalId
  identifier for the current evaluation, which may differ from the evaluation counters in the case of evaluation scheduling; used on iterator master as well as server processors. Currently, this is set prior to all invocations of derived_map() for all processors.

• bool fineGrainEvalCounters
  controls use of fn val/grad/hess counters for detailed evaluation report

• int evalIdCntr
  total interface evaluation counter

• int newEvalIdCntr
  new (non-duplicate) interface evaluation counter

• int evalIdRefPt
  iteration reference point for evalIdCntr

• int newEvalIdRefPt
  iteration reference point for newEvalIdCntr

• IntArray fnValCounter
  number of value evaluations by resp fn

• IntArray fnGradCounter
  number of gradient evaluations by resp fn

• IntArray fnHessCounter
  number of Hessian evaluations by resp fn

• IntArray newFnValCounter
  number of new value evaluations by resp fn

• IntArray newFnGradCounter
  number of new gradient evaluations by resp fn
• IntArray **newFnHessCounter**
  number of new Hessian evaluations by resp fn
• IntArray **fnValRefPt**
  iteration reference point for fnValCounter
• IntArray **fnGradRefPt**
  iteration reference point for fnGradCounter
• IntArray **fnHessRefPt**
  iteration reference point for fnHessCounter
• IntArray **newFnValRefPt**
  iteration reference point for newFnValCounter
• IntArray **newFnGradRefPt**
  iteration reference point for newFnGradCounter
• IntArray **newFnHessRefPt**
  iteration reference point for newFnHessCounter
• IntResponseMap **rawResponseMap**
  Set of responses returned by either a blocking or nonblocking schedule.
• IntResponseMap **cachedResponseMap**
  Set of available asynchronous responses completed within a blocking or nonblocking scheduler that cannot be
  processed in a higher level context and need to be stored for later.
• StringArray **fnLabels**
  response function descriptors (used in print_evaluation_summary() and derived direct interface classes); initialized
  in map() functions due to potential updates after construction
• bool **multiProcEvalFlag**
  flag for multiprocessor evaluation partitions (evalComm)
• bool **ieDedMasterFlag**
  flag for dedicated master partitioning at the iterator level
• String **evalTagPrefix**
  set of period-delimited evaluation ID tags to use in evaluation tagging
• bool **appendIfaceId**
  whether to append the interface ID to the prefix during map (default true)

**Private Member Functions**

• Interface * **get_interface** (ProblemDescDB &problem_db)
  Used by the envelope to instantiate the correct letter class.
• int **algebraic_function_type** (String)
  Used by algebraic mappings to determine the correct AMPL function evaluation call to make.

**Private Attributes**

• StringArray **algebraicVarTags**
  set of variable tags from AMPL stub.col
• SizetArray **algebraicACVIndices**
  set of indices mapping AMPL algebraic variables to DAKOTA all continuous variables
• SizetArray algebraicACVIds
  set of ids mapping AMPL algebraic variables to DAKOTA all continuous variables
• StringArray algebraicFnTags
  set of function tags from AMPL stub.row
• IntArray algebraicFnTypes
  function type: \( > 0 = \text{objective}, < 0 = \text{constraint} \) \(|\text{value}|-1\) is the objective (constraint) index when making AMPL 
  objval (conival) calls
• SizetArray algebraicFnIndices
  set of indices mapping AMPL algebraic objective functions to DAKOTA response functions
• RealArray algebraicConstraintWeights
  set of weights for computing Hessian matrices for algebraic constraints;
• int numAlgebraicResponses
  number of algebraic responses (objectives+constraints)
• Interface * interfaceRep
  pointer to the letter (initialized only for the envelope)
• int referenceCount
  number of objects sharing interfaceRep
• ASL * asl
  pointer to an AMPL solver library (ASL) object

### 13.66.1 Detailed Description

Base class for the interface class hierarchy.

The Interface class hierarchy provides the part of a Model that is responsible for mapping a set of Variables into a set of Responses. The mapping is performed using either a simulation-based application interface or a surrogate-based approximation interface. For memory efficiency and enhanced polymorphism, the interface hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Interface) serves as the envelope and one of the derived classes (selected in Interface::get_interface()) serves as the letter.

### 13.66.2 Constructor & Destructor Documentation

**Interface ( )**

default constructor
  used in Model envelope class instantiations

**Interface ( ProblemDescDB & problem_db )**

standard constructor for envelope
  Used in Model instantiation to build the envelope. This constructor only needs to extract enough data to properly execute get_interface, since Interface::Interface(BaseConstructor, problem_db) builds the actual base class data inherited by the derived interfaces.
  References Dakota::abort_handler(), Interface::get_interface(), and Interface::interfaceRep.
CHAPTER 13. CLASS DOCUMENTATION

**Interface** ( const Interface & interface )

copy constructor

Copy constructor manages sharing of interfaceRep and incrementing of referenceCount.
References Interface::interfaceRep, and Interface::referenceCount.

**~Interface** ( ) [virtual]
destructor

Destructor decrements referenceCount and only deletes interfaceRep if referenceCount is zero.
References Interface::interfaceRep, and Interface::referenceCount.

**Interface** ( BaseConstructor, const ProblemDescDB & problem ) [protected]
constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all inherited interfaces. **get_interface()** instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid the recursion of the base class constructor calling get_interface() again). Since this is the letter and the letter IS the representation, interfaceRep is set to NULL (an uninitialized pointer causes problems in ~Interface).

References Dakota::abort_handler(), Interface::algebraic_function_type(), Interface::algebraicConstraintWeights, Interface::algebraicFnTags, Interface::algebraicFnTypes, Interface::algebraicMappings, Interface::algebraicVarTags, Interface::asl, ProblemDescDB::get_string(), Interface::outputLevel, and Dakota::strends().

### 13.66.3 Member Function Documentation

**Interface operator=( const Interface & interface )**

assignment operator


References Interface::interfaceRep, and Interface::referenceCount.

**void assign_rep ( Interface * interface_rep, bool ref_count_incr = true )**

assign letter or replace existing letter with a new one

Similar to the assignment operator, the **assign_rep()** function decrements referenceCount for the old interface-Rep and assigns the new interfaceRep. It is different in that it is used for publishing derived class letters to existing envelopes, as opposed to sharing representations among multiple envelopes (in particular, assign_rep is passed a letter object and operator= is passed an envelope object). Letter assignment supports two models as governed by ref_count_incr:

- ref_count_incr = true (default): the incoming letter belongs to another envelope. In this case, increment the reference count in the normal manner so that deallocation of the letter is handled properly.
- ref_count_incr = false: the incoming letter is instantiated on the fly and has no envelope. This case is modeled after **get_interface()**: a letter is dynamically allocated using new and passed into assign_rep, the letter’s reference count is not incremented, and the letter is not remotely deleted (its memory management is passed over to the envelope).

References Dakota::abort_handler(), Interface::interfaceRep, and Interface::referenceCount.

Reference by DataFitSurrModel::DataFitSurrModel(), parallel_interface_plugin(), LibraryEnvironment::plugin_interface(), and run_dakota().
void eval_tag_prefix ( const String & eval_id_str, bool append_iface_id = true )
set the evaluation tag prefix (does not recurse)
    default implementation just sets the list of eval ID tags; derived classes containing additional models or interfaces should override (currently no use cases)
    References Interface::append_ifaceId, Interface::eval_tag_prefix(), Interface::evalTagPrefix, and Interface::interface-Rep.
    Referenced by NestedModel::derived_evaluate(), SimulationModel::eval_tag_prefix(), and Interface::eval_tag_prefix().

void response_mapping ( const Response & algebraic_response, const Response & core_response, Response & total_response ) [protected]
combine the response from algebraic_mappings() with the response from derived_map() to create the total response
    This function will get invoked even when only algebraic mappings are active (no core mappings from derived_map), since the AMPL algebraic_response may be ordered differently from the total_response. In this case, the core_response object is unused.
    References Dakota::NPOS, Dakota::abort_handler(), Response::active_set_derivative_vector(), Response::active_set_request_vector(), Interface::algebraicACVIds, Interface::algebraicFnIndices, Interface::coreMappings, Dakota::find_index(), Response::function_gradient(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian(), Response::function_hessian_view(), Response::function_hessians(), Response::function_value(), Response::function_values(), Response::function_values_view(), Interface::outputLevel, Response::reset(), and Response::reset_inactive().
    Referenced by ApproximationInterface::map(), ApplicationInterface::map(), ApplicationInterface::synchronize(), and ApplicationInterface::synchronize_nowait().

Interface * get_interface ( ProblemDescDB & problem_db ) [private]
Used by the envelope to instantiate the correct letter class.
    used only by the envelope constructor to initialize interfaceRep to the appropriate derived type.
    References ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), and Interface::interface_type().
    Referenced by Interface::Interface().

13.66.4 Member Data Documentation

IntResponseMap rawResponseMap [protected]
Set of responses returned by either a blocking or nonblocking schedule.
    The map is a full/partial set of completions which are identified through their evalIdCntr key. The raw set is postprocessed (i.e., finite diff grads merged) in Model::synchronize() where it becomes responseMap.
    Referenced by ApplicationInterface::asynchronous_local_evaluations(), Interface::cache_unmatched_response(), ApplicationInterface::process_asynch_local(), ApplicationInterface::process_sync_local(), ApplicationInterface::receive_evaluation(), ApplicationInterface::synchronize(), ApproximationInterface::synchronize(), ApplicationInterface::synchronize_nowait(), ApproximationInterface::synchronize_nowait(), ApplicationInterface::test_local_backfill(), and ApplicationInterface::testreceives_backfill().
    The documentation for this class was generated from the following files:
    - DakotaInterface.hpp
    - DakotaInterface.cpp
13.67 Iterator Class Reference

Base class for the iterator class hierarchy.

Inheritance diagram for Iterator:

```
Iterator
|     | MetaIterator
|     | Minimizer
|     | NonD
|     | PStudyDACE
|     | Verification
|     | Analyzer
|     | CollabHybridMetaIterator
|     | ConcurrentMetaIterator
|     | EmbedHybridMetaIterator
|     | SeqHybridMetaIterator
|     | LeastSq
|     | Optimizer
|     | PebbldMinimizer
|     | SurrBasedMinimizer
```

**Public Member Functions**

- **Iterator ()**
  - default constructor
- **Iterator (Iterator *iterator_rep, bool ref_count_incr=true)**
  - alternate envelope constructor that assigns a representation pointer
- **Iterator (ProblemDescDB &problem_db)**
  - standard envelope constructor, which constructs its own model(s)
- **Iterator (ProblemDescDB &problem_db, Model &model)**
  - alternate envelope constructor which uses the ProblemDescDB but accepts a model from a higher level (meta-iterator) context, instead of constructing its own
- **Iterator (const String &method_string, Model &model)**
  - alternate envelope constructor for instantiations by name without the ProblemDescDB
- **Iterator (const Iterator &iterator)**
  - copy constructor
- **virtual ~Iterator ()**
  - destructor
- **Iterator operator= (const Iterator &iterator)**
  - assignment operator
- **virtual void derived_set_communicators (ParLevLIter pl_iter)**
  - derived class contributions to setting the communicators associated with this Iterator instance
- **virtual void derived_free_communicators (ParLevLIter pl_iter)**
  - derived class contributions to freeing the communicators associated with this Iterator instance
- **virtual void initialize_run ()**
  - utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
- **virtual void pre_run ()**
  - pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- **virtual void core_run ()**
  - core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
• virtual void post_run (std::ostream &s)
  
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

• virtual void finalize_run ()

  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

• virtual void pre_output ()
  write variables to file, following pre-run

• virtual void post_input ()
  read tabular data for post-run mode

• virtual void reset ()
  restore initial state for repeated sub-iterator executions

• virtual void initialize_iterator (int job_index)
  used by IteratorScheduler to set the starting data for a run

• virtual void pack_parameters_buffer (MPIPackBuffer &send_buffer, int job_index)
  used by IteratorScheduler to pack starting data for an iterator run

• virtual void unpack_parameters_buffer (MPIUnpackBuffer &recv_buffer, int job_index)
  used by IteratorScheduler to unpack starting data for an iterator run

• virtual void unpack_parameters_initialize (MPIUnpackBuffer &recv_buffer, int job_index)
  used by IteratorScheduler to unpack starting data and initialize an iterator run

• virtual void pack_results_buffer (MPIPackBuffer &send_buffer, int job_index)
  used by IteratorScheduler to pack results data from an iterator run

• virtual void unpack_results_buffer (MPIUnpackBuffer &recv_buffer, int job_index)
  used by IteratorScheduler to unpack results data from an iterator run

• virtual void update_local_results (int job_index)
  used by IteratorScheduler to update local results arrays

• virtual const Variables & variables_results () const
  return a single final iterator solution (variables)

• virtual const Response & response_results () const
  return a single final iterator solution (response)

• virtual const VariablesArray & variables_array_results ()
  return multiple final iterator solutions (variables). This should only be used if returns_multiple_points() returns true.

• virtual const ResponseArray & response_array_results ()
  return multiple final iterator solutions (response). This should only be used if returns_multiple_points() returns true.

• virtual void response_results_active_set (const ActiveSet &set)
  set the requested data for the final iterator response results

• virtual const RealVector & response_error_estimates () const
  return error estimates associated with the final iterator solution

• virtual bool accepts_multiple_points () const
  indicates if this iterator accepts multiple initial points. Default return is false. Override to return true if appropriate.

• virtual bool returns_multiple_points () const
  indicates if this iterator returns multiple final points. Default return is false. Override to return true if appropriate.

• virtual void initial_points (const VariablesArray &pts)
sets the multiple initial points for this iterator. This should only be used if `accepts_multiple_points()` returns true.

- virtual void initialize_graphics (int iterator_server_id=1)
  initialize the 2D graphics window and the tabular graphics data
- virtual void print_results (std::ostream &s)
  print the final iterator results
- virtual const Model & algorithm_space_model () const
  return the result of any recasting or surrogate model recursion layered on top of iteratedModel by the derived Iterator ctor chain
- virtual unsigned short uses_method () const
  return name of any enabling iterator used by this iterator
- virtual void method_recourse ()
  perform a method switch, if possible, due to a detected conflict
- virtual const VariablesArray & all_variables ()
  return the complete set of evaluated variables
- virtual const RealMatrix & all_samples ()
  return the complete set of evaluated samples
- virtual const IntResponseMap & all_responses () const
  return the complete set of computed responses
- virtual int num_samples () const
  get the current number of samples
- virtual void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)
  reset sampling iterator to use at least min_samples
- virtual void sampling_reference (int samples_ref)
  set reference number of samples, which is a lower bound during reset
- virtual void sampling_increment ()
  increment to next in sequence of refinement samples
- virtual unsigned short sampling_scheme () const
  return sampling name
- virtual bool compact_mode () const
  returns `Analyzer::compactMode`
- virtual IntIntPair estimate_partition_bounds ()
  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- virtual bool resize ()
  reinitializes iterator based on new variable size
- void init_communicators (ParLevLIter pl_iter)
  initialize the communicators associated with this Iterator instance
- void set_communicators (ParLevLIter pl_iter)
  set the communicators associated with this Iterator instance
- void free_communicators (ParLevLIter pl_iter)
  free the communicators associated with this Iterator instance
- void resize_communicators (ParLevLIter pl_iter, bool reinit_comms)
  Resize the communicators. This is called from the letter’s `resize()`
- void parallel_configuration_iterator (ParConfigLIter pc_iter)
set methodPCIter

- ParConfigLIter parallel_configuration_iterator () const
  return methodPCIter
- void run (ParLevLIter pl_iter)
  invoke set_communicators(pl_iter) prior to run()
- void run ()
  orchestrate initialize/pre/core/post/finalize phases
- void assign_rep (Iterator *iterator_rep, bool ref_count_incr=true)
  replaces existing letter with a new one
- void iterated_model (const Model &model)
  set the iteratedModel (iterators and meta-iterators using a single model instance)
- Model & iterated_model ()
  return the iteratedModel (iterators & meta-iterators using a single model instance)
- ProblemDescDB & problem_description_db () const
  return the problem description database (probDescDB)
- ParallelLibrary & parallel_library () const
  return the parallel library (parallelLib)
- void method_name (unsigned short m_name)
  set the method name to an enumeration value
- unsigned short method_name () const
  return the method name via its native enumeration value
- void method_string (const String &m_str)
  set the method name by string
- String method_string () const
  return the method name by string
- String method_enum_to_string (unsigned short method_name) const
  convert a method name enumeration value to a string
- unsigned short method_string_to_enum (const String &method_name) const
  convert a method name string to an enumeration value
- String submethod_enum_to_string (unsigned short submethod_name) const
  convert a method name enumeration value to a string
- const String & method_id () const
  return the method identifier (methodId)
- int maximum_evaluation_concurrency () const
  return the maximum evaluation concurrency supported by the iterator
- void maximum_evaluation_concurrency (int max_conc)
  set the maximum evaluation concurrency supported by the iterator
- int maximum_iterations () const
  return the maximum iterations for this iterator
- void maximum_iterations (int max_iter)
  set the maximum iterations for this iterator
- void convergence_tolerance (Real conv_tol)
  set the method convergence tolerance (convergenceTol)
Real convergence_tolerance () const

return the method convergence tolerance (convergenceTol)

void output_level (short out_lev)

set the method output level (outputLevel)

short output_level () const

return the method output level (outputLevel)

void summary_output (bool summary_output_flag)

Set summary output control; true enables evaluation/results summary.

size_t num_final_solutions () const

return the number of solutions to retain in best variables/response arrays

void num_final_solutions (size_t num_final)

set the number of solutions to retain in best variables/response arrays

void active_set (const ActiveSet &set)

set the default active set vector (for use with iterators that employ evaluate_parameter_sets())

const ActiveSet & active_set () const

return the default active set vector (used by iterators that employ evaluate_parameter_sets())

void sub_iterator_flag (bool si_flag)

set subIteratorFlag (and update summaryOutputFlag if needed)

void active_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

set primaryA {CV, DIV, DRV} MapIndices, secondaryA {CV, DIV, DRV} MapTargets

bool is_null () const

function to check iteratorRep (does this envelope contain a letter?)

Iterator * iterator_rep () const

returns iteratorRep for access to derived class member functions that are not mapped to the top Iterator level

virtual void eval_tag_prefix (const String &eval_id_str)

set the hierarchical eval ID tag prefix

Protected Member Functions

Iterator (BaseConstructor, ProblemDescDB &problem_db)

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

Iterator (NoDBBaseConstructor, unsigned short method_name, Model &model)

alternate constructor for base iterator classes constructed on the fly

Iterator (NoDBBaseConstructor, unsigned short method_name)

alternate constructor for base iterator classes constructed on the fly

virtual void derived_init_communicators (ParLevLIter pl_iter)

derived class contributions to initializing the communicators associated with this Iterator instance

virtual void update_from_model (const Model &model)

set inherited data attributes based on extractions from incoming model

virtual const VariablesArray & initial_points () const

gets the multiple initial points for this iterator. This will only be meaningful after a call to initial_points mutator.

StrStrSizet run_identifier () const

get the unique run identifier based on method name, id, and number of executions
Static Protected Member Functions

- static void gnewton_set_recast (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)
  conversion of request vector values for the Gauss-Newton Hessian approximation

Protected Attributes

- ProblemDescDB & probDescDB
  class member reference to the problem description database
- ParallelLibrary & parallelLib
  class member reference to the parallel library
- ParConfigLIter methodPCIter
  the active ParallelConfiguration used by this Iterator instance
- Model iteratedModel
  the model to be iterated (for iterators and meta-iterators employing a single model instance)
- size_t myModelLayers
  number of Models locally (in Iterator or derived classes) wrapped around the initially passed in Model
- unsigned short methodName
  name of the iterator (the user’s method spec)
- Real convergenceTol
  iteration convergence tolerance
- int maxIterations
  maximum number of iterations for the iterator
- int maxFunctionEvals
  maximum number of fn evaluations for the iterator
- int maxEvalConcurrency
  maximum number of concurrent model evaluations
- ActiveSet activeSet
  the response data requirements on each function evaluation
- size_t numFinalSolutions
  number of solutions to retain in best variables/response arrays
- VariablesArray bestVariablesArray
  collection of N best solution variables found during the study; always in context of Model originally passed to the Iterator (any in-flight Recasts must be undone)
- ResponseArray bestResponseArray
  collection of N best solution responses found during the study; always in context of Model originally passed to the Iterator (any in-flight Recasts must be undone)
- bool subIteratorFlag
  flag indicating if this Iterator is a sub-iterator (NestedModel::subIterator or DataFitSurrModel::daceIterator)
- SizetArray primaryACVarMapIndices
  “primary” all continuous variable mapping indices flowed down from higher level iteration
- SizetArray primaryADIVarMapIndices
  “primary” all discrete int variable mapping indices flowed down from higher level iteration
- SizetArray primaryADSVarMapIndices
"primary" all discrete string variable mapping indices flowed down from higher level iteration

- `SizetArray primaryADRVarMapIndices`

"primary" all discrete real variable mapping indices flowed down from higher level iteration

- `ShortArray secondaryACVarMapTargets`

"secondary" all continuous variable mapping targets flowed down from higher level iteration

- `ShortArray secondaryADIVarMapTargets`

"secondary" all discrete int variable mapping targets flowed down from higher level iteration

- `ShortArray secondaryADSVarMapTargets`

"secondary" all discrete string variable mapping targets flowed down from higher level iteration

- `ShortArray secondaryADRVarMapTargets`

\[\text{short outputLevel}\]

output verbosity level: \{SILENT, QUIET, NORMAL, VERBOSE, DEBUG\}_OUTPUT

- `bool summaryOutputFlag`

flag for summary output (evaluation stats, final results); default true, but false for on-the-fly (helper) iterators and sub-iterator use cases

- `ResultsManager & resultsDB`

reference to the global iterator results database

- `ResultsNames resultsNames`

valid names for iterator results

**Private Member Functions**

- `Iterator * get_iterator (ProblemDescDB &problem_db)`
  
  Used by the envelope to instantiate the correct letter class.

- `Iterator * get_iterator (ProblemDescDB &problem_db, Model &model)`
  
  Used by the envelope to instantiate the correct letter class.

- `Iterator * get_iterator (const String &method_string, Model &model)`
  
  Used by the envelope to instantiate the correct letter class.

**Private Attributes**

- `String methodId`

  method identifier string from the input file

- `size_t execNum`

  an execution number for this instance of the class, unique across all instances of same methodName/methodId

- std::map< size_t, ParConfigLIter > methodPCIterMap

  track the available configurations that have been created (init_communicators) and are available for activation at run time (set_communicators)

- `Iterator * iteratorRep`

  pointer to the letter (initialized only for the envelope)

- `int referenceCount`

  number of objects sharing iteratorRep
13.67. ITERATOR CLASS REFERENCE

13.67.1 Detailed Description

Base class for the iterator class hierarchy.

The Iterator class is the base class for one of the primary class hierarchies in DAKOTA. The iterator hierarchy contains all of the iterative algorithms which use repeated execution of simulations as function evaluations. For memory efficiency and enhanced polymorphism, the iterator hierarchy employs the “letter/envelope idiom” (see Coplien ”Advanced C++”, p. 133), for which the base class (Iterator) serves as the envelope and one of the derived classes (selected in Iterator::get_iterator()) serves as the letter.

13.67.2 Constructor & Destructor Documentation

Iterator ( )

default constructor

The default constructor is used in Vector<Iterator> instantiations and for initialization of Iterator objects contained in meta-Iterators and Model recursions. iteratorRep is NULL in this case, making it necessary to check for NULL pointers in the copy constructor, assignment operator, and destructor.

Iterator ( Iterator * iterator_rep, bool ref_count_incr = true )

alternate envelope constructor that assigns a representation pointer

This constructor assigns a representation pointer and optionally increments its reference count. It behaves the same as a default construction followed by assign_rep().

References Iterator::iteratorRep, and Iterator::referenceCount.

Iterator ( ProblemDescDB & problem_db )

standard envelope constructor, which constructs its own model(s)

Envelope constructor only needs to extract enough data to properly execute get_iterator(), since letter holds the actual base class data. This version is used for top-level ProblemDescDB-driven construction of all Iterators and MetaIterators, which construct their own Model instances.

References Dakota::abort_handler(), Iterator::get_iterator(), and Iterator::iteratorRep.

Iterator ( ProblemDescDB & problem_db, Model & model )

alternate envelope constructor which uses the ProblemDescDB but accepts a model from a higher level (meta-iterator) context, instead of constructing its own

Envelope constructor only needs to extract enough data to properly execute get_iterator(), since letter holds the actual base class data. This version is used for ProblemDescDB-driven construction of Iterators that are passed a Model from a higher-level context (e.g., a MetaIterator instantiates its sub-iterator(s) by name instead of pointer and passes in its iteratedModel, since these sub-iterators lack their own model pointers).

References Dakota::abort_handler(), Iterator::get_iterator(), and Iterator::iteratorRep.

Iterator ( const String & method_string, Model & model )

alternate envelope constructor for instantiations by name without the ProblemDescDB

Used in sub-iterator instantiations within iterator constructors. Envelope constructor only needs to extract enough data to properly execute get_iterator(), since letter holds the actual base class data. This version is used for lightweight constructions without the ProblemDescDB.

References Dakota::abort_handler(), Iterator::get_iterator(), and Iterator::iteratorRep.
**Iterator ( const Iterator & iterator )**

Copy constructor
- Copy constructor manages sharing of iteratorRep and incrementing of referenceCount.
- References Iterator::iteratorRep, and Iterator::referenceCount.

**~Iterator ( ) [virtual]**

Destructor
- Destructor decrements referenceCount and only deletes iteratorRep when referenceCount reaches zero.
- References Iterator::iteratorRep, and Iterator::referenceCount.

**Iterator ( BaseConstructor , ProblemDescDB & problem_db ) [protected]**

Constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- This constructor builds the base class data for all inherited iterators, including meta-iterators. get_iterator() instantiates a derived class and the derived class selects this base class constructor in its initialization list (to avoid the recursion of the base class constructor calling get_iterator() again). Since the letter IS the representation, its representation pointer is set to NULL (an uninitialized pointer causes problems in ~Iterator).
- References Iterator::method_enum_to_string(), Iterator::methodName, and Iterator::outputLevel.

**Iterator ( NoDBBaseConstructor , unsigned short method_name , Model & model ) [protected]**

Alternate constructor for base iterator classes constructed on the fly
- This alternate constructor builds base class data for inherited iterators. It is used for on-the-fly instantiations for which DB queries cannot be used, and is not used for construction of meta-iterators.

**Iterator ( NoDBBaseConstructor , unsigned short method_name ) [protected]**

Alternate constructor for base iterator classes constructed on the fly
- This alternate constructor builds base class data for inherited iterators. It is used for on-the-fly instantiations for which DB queries cannot be used, and is not used for construction of meta-iterators. It has no incoming model, so only sets up a minimal set of defaults. However, its use is preferable to the default constructor, which should remain as minimal as possible.

**13.67.3 Member Function Documentation**

**Iterator operator= ( const Iterator & iterator )**

Assignment operator
- References Iterator::iteratorRep, and Iterator::referenceCount.

**void initialize_run ( ) [virtual]**

Utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
- Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s initialize_run(), typically before performing its own implementation steps.
void pre_run( )  [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

void core_run( )  [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post run function for the iterator class hierarchy. All derived classes need to redefine it.

void post_run( std::ostream & s )  [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

References Iterator::initialize_run(), and Iterator::iteratorRep.

References Dakota::abort_handler(), Iterator::core_run(), and Iterator::iteratorRep.

References Iterator::core_run(), and Iterator::iteratorRep.

References Iterator::post_run(), and Iterator::run().

References Iterator::pre_run(), and Iterator::run().

References Iterator::iteratorRep, and Iterator::pre_run().

References Iterator::iteratorRep, and Iterator::post_run().

References Iterator::pre_run(), and Iterator::run().

References Iterator::iteratorRep, and Iterator::run().

References Iterator::pre_run(), and Iterator::run().

References Iterator::iteratorRep, and Iterator::run().
void finalize_run() [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s finalize_run(), typically after performing its own implementation steps.
Reimplemented in NonD, SNLLOptimizer, Analyzer, Minimizer, SNLLLeastSq, Optimizer, and LeastSq.
References Iterator::finalize_run(), and Iterator::iteratorRep.
Referenced by Iterator::finalize_run(), Minimizer::finalize_run(), Analyzer::finalize_run(), Iterator::run(), and SeqHybridMetaIterator::run_sequential()

void initialize_graphics(int iterator_server_id = 1) [virtual]

initialize the 2D graphics window and the tabular graphics data
This is a convenience function for encapsulating graphics initialization operations. It is overridden by derived classes that specialize the graphics display.
Reimplemented in NonDReliability, and SurrBasedMinimizer.
References Model::auto_graphics(), Graphics::create_plots_2d(), OutputManager::create_tabular_datastream(),
Model::current_response(), Model::current_variables(), OutputManager::graph2DFlag, OutputManager::graphics(),
Iterator::initialize_graphics(), Iterator::iteratedModel, Iterator::iteratorRep, ParallelLibrary::output_manager(), Iterator::parallelLib, and OutputManager::tabularDataFlag.
Referenced by CollabHybridMetaIterator::core_run(), EmbedHybridMetaIterator::core_run(), ConcurrentMetaIterator::core_run(), Environment::execute(), Iterator::initialize_graphics(), SeqHybridMetaIterator::run_sequential(),
and SeqHybridMetaIterator::run_sequential()

void print_results(std::ostream & s) [virtual]

print the final iterator results
This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().
Reimplemented in Analyzer, NonDGPMSABayesCalibration, NonDLHSSampling, NonDPolynomialChaos,
NonDBayesCalibration, NonDDREAMBayesCalibration, NonDPOFDarts, NonDLocalReliability, NonDWAASABayesCalibration,
NonDQUESOBayesCalibration, SeqHybridMetaIterator, NonDAdaptiveSampling, ConcurrentMetaIterator,
NonDGPIMpsampling, Optimizer, NonDAdaptImpSampling, NonDExpansion, NonDInterval, NonDMultilevelSampling,
PStudyDACE, LeastSq, Verification, NonDGlobalReliability, SurrBasedMinimizer, RichExtrapVerification,
and PebblIDMinimizer.
References Iterator::iteratorRep, and Iterator::print_results().
Referenced by MetaIterator::post_run(), Minimizer::post_run(), and Iterator::print_results().

unsigned short uses_method() const [virtual]

return name of any enabling iterator used by this iterator
This is used to avoid clashes in state between non-object-oriented (i.e., F77, C) iterator executions, when such iterators could potentially be executing simultaneously (e.g., nested execution). It is not an issue (and a used method is not reported) in cases where a helper execution is completed before a lower level one could be initiated; an example of this is DIRECT for maximization of expected improvement: the EIF maximization is completed before a new point evaluation (which could include nested iteration) is performed.
Reimplemented in NonDLocalReliability, and NonDLocalInterval.
References Iterator::iteratorRep, and Iterator::uses_method().
Referenced by DOTOptimizer::initialize(), CONMINOptimizer::initialize(), NCSUOptimizer::initialize(), NL-PQLPoptimizer::initialize(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), SOLBase::SOLBase(), and Iterator::uses_method().

```cpp
void run ( )
```

Orchestrate initialize/pre/core/post/finalize phases.

Iterator supports a construct/initialize-run/pre-run/core-run/post-run/finalize-run/destruct progression. This member (non-virtual) function sequences these run phases.

References ParallelLibrary::command_line_post_run(), ParallelLibrary::command_line_pre_run(), ParallelLibrary::command_line_run(), Iterator::core_run(), Iterator::execNum, Iterator::finalize_run(), ResultsID::increment_id(), Iterator::initialize_run(), ResultsID::instance(), Iterator::iteratorRep, Iterator::method_enum_to_string(), Iterator::method_id(), Iterator::method_string(), Iterator::methodName, Iterator::outputLevel, Iterator::parallelLib, Iterator::post_input(), Iterator::post_run(), Iterator::pre_output(), Iterator::pre_run(), Iterator::run(), and Iterator::summary_OutputFlag.

Referenced by Iterator::run().

```cpp
void assign_rep ( Iterator * iterator_rep, bool ref_count_incr = true )
```

Replaces existing letter with a new one.

Similar to the assignment operator, the assign_rep() function decrements referenceCount for the old iteratorRep and assigns the new iteratorRep. It is different in that it is used for publishing derived class letters to existing envelopes, as opposed to sharing representations among multiple envelopes (in particular, assign_rep is passed a letter object and operator= is passed an envelope object). Letter assignment supports two models as governed by ref_count_incr:

- **ref_count_incr = true** (default): the incoming letter belongs to another envelope. In this case, increment the reference count in the normal manner so that deallocation of the letter is handled properly.

- **ref_count_incr = false**: the incoming letter is instantiated on the fly and has no envelope. This case is modeled after get_iterator(): a letter is dynamically allocated using new and passed into assign_rep, the letter’s reference count is not incremented, and the letter is not remotely deleted (its memory management is passed over to the envelope).

References Dakota::abort_handler(), Iterator::iterator_rep(), Iterator::iteratorRep, and Iterator::referenceCount.

Referenced by NonDBayesCalibration::calibrate_to_hifi(), NonDExpansion::construct_cubature(), NonDExpansion::construct_expansion_sampler(), NonDAdaptiveSampling::construct_fsu_sampler(), NonD::construct_lhs(), NonDBayesCalibration::construct_map_optimizer(), NonDBayesCalibration::construct_mcmc_model(), NonDExpansion::construct_quadrature(), NonDExpansion::construct_sparse_grid(), Minimizer::data_transform_model(), EffGlobalMinimizer::EffGlobalMinimizer(), ActiveSubspaceModel::init_fullspace_sampler(), NonDLocalInterval::method_recourse(), NonDLocalReliability::method_recourse(), NonDAdaptiveSampling::NonDAdaptiveSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDGPlmpSampling::NonDGPlmpSampling(), NonDGPlmpSampling(), NonDGPM SabhaSbayesCalibration::NonDGPM SabhaSbayesCalibration(), NonDLHSInterval::NonDLHSInterval(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), GaussProcApproximation::optimize_theta_global(), GaussProcApproximation::optimize_theta_multipoint(), and SurrBasedLocalMinimizer::relax_constraints().

```cpp
void eval_tag_prefix ( const String & eval_id_str ) [virtual]
```

Set the hierarchical eval ID tag prefix.
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This prepend may need to become a virtual function if the tagging should propagate to other subModels or helper Iterators an Iterator may contain.

References Iterator::eval_tag_prefix(), Model::eval_tag_prefix(), Iterator::iteratedModel, and Iterator::iterator-Rep.

Referenced by NestedModel::derived_evaluate(), Iterator::eval_tag_prefix(), Iterator::init_communicators(), NestedModel::initialize_iterator(), and DataFitSurrModel::run_dace_iterator().

```cpp
void gnewton_set_recast ( const Variables & recast_vars, const ActiveSet & recast_set, ActiveSet & sub_model_set ) [static], [protected]
```

conversion of request vector values for the Gauss-Newton Hessian approximation

For Gauss-Newton Hessian requests, activate the 2 bit and mask the 4 bit.

References ActiveSet::request_value(), and ActiveSet::request_vector().

Referenced by NonDBayesCalibration::construct_map_optimizer(), and Optimizer::reduce_model().

```cpp
Iterator * get_iterator ( ProblemDescDB & problem_db ) [private]
```

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize iteratorRep to the appropriate derived type, as given by the DB’s method_name. Supports all iterators and meta-iterators. These instantiations will NOT recurse on the Iterator(problem_db) constructor due to the use of BaseConstructor.

References ProblemDescDB::get_model(), ProblemDescDB::get_ushort(), Iterator::method_enum_to_string(), Iterator::method_name(), and Dakota::SUBMETHOD_COLLABORATIVE.

Referenced by Iterator::Iterator().

```cpp
Iterator * get_iterator ( ProblemDescDB & problem_db, Model & model ) [private]
```

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize iteratorRep to the appropriate derived type. Alternate construction of meta-iterators is supported to enable use of meta-iterators as components. These instantiations will NOT recurse on the Iterator(problem_db, model) constructor due to the use of BaseConstructor.

References ProblemDescDB::get_ushort(), Iterator::method_enum_to_string(), Iterator::method_name(), Iterator::probDescDB, Dakota::SUBMETHOD_COLLABORATIVE, and Model::surrogate_type().

```cpp
Iterator * get_iterator ( const String & method_string, Model & model ) [private]
```

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize iteratorRep to the appropriate derived type, as given by the passed method_string. Lightweight instantiations by name are supported by a subset of Iterators (primarily Minimizers).

References Dakota::strbegins(), and Dakota::strends().

13.67.4 Member Data Documentation

ProblemDescDB& probDescDB [protected]

class member reference to the problem description database

Iterator and Model cannot use a shallow copy of ProblemDescDB due to circular destruction dependency (reference counts can’t get to 0), since ProblemDescDB contains {iterator,model}List.
Referenced by MetaIterator::allocate_by_name(), MetaIterator::allocate_by_pointer(), Analyzer::Analyzer(), MetaIterator::check_model(), COLINOptimizer::COLINOptimizer(), NonDBayesCalibration::construct_mcmc_model(), Minimizer::data_transform_model(), DataFitSurrBasedLocalMinimizer::DataFitSurrBasedLocalMinimizer(), SurrBasedMinimizer::derived_init_communicators(), EmbedHybridMetaIterator::derived_init_communicators(), ConcurrentMetaIterator::derived_init_communicators(), EffGlobalMinimizer::EffGlobalMinimizer(), MetaIterator::estimate_by_name(), MetaIterator::estimate_by_pointer(), CollabHybridMetaIterator::estimate_partition_bounds(), EmbedHybridMetaIterator::estimate_partition_bounds(), ConcurrentMetaIterator::estimate_partition_bounds(), SeqHybridMetaIterator::estimate_partition_bounds(), FSUDesignCompExp::FSUDesignCompExp(), Iterator::get_iterator(), HierarchSurrBasedLocalMinimizer::HierarchSurrBasedLocalMinimizer(), ConcurrentMetaIterator::init_model(), NOWPACOptimizer::initialize_options(), SurrBasedLocalMinimizer::initialize_sub_minimizer(), JEGAOptimizer::JEGAOptimizer(), NLSSOLVEstSq::NLSSOLVEstSq(), NomadOptimizer::NomadOptimizer(), NonD::NonD(), NonDAdaptImpSampling::NonDAdaptImpSampling(), NonDAdaptiveSampling::NonDAdaptiveSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDGImpSampling::NonDGImpSampling(), NonDGPSABCayesCalibration::NonDGPSABCayesCalibration(), NonDGPMSABCayesCalibration::NonDGPMSABCayesCalibration(), NonDInterval::NonDInterval(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), NonDPolynomialChaos::NonDPolynomialChaos(), NonDQuadature::NonDQuadature(), NonDSampling::NonDSampling(), NonDSParseGrid::NonDSParseGrid(), NonDStochCollocation::NonDStochCollocation(), NPSOLOptimizer::NPSOLOptimizer(), OptDartsOptimizer::OptDartsOptimizer(), ParamStudy::ParamStudy(), NonlinearCGOptimizer::parse_options(), NonDAdaptImpSampling::parse_options(), PebblMinimizer::PebblMinimizer(), Iterator::problem_description_db(), APPSOptimizer::set_apps_parameters(), COLINOptimizer::set_solver_parameters(), SNLLLeastSq::SNLLLeastSq(), SNLOptimizer::SNLOptimizer(), COLINOptimizer::solver_setup(), and SurrBasedGlobalMinimizer::SurrBasedGlobalMinimizer().

int maxEvalConcurrency [protected]

maximum number of concurrent model evaluations

This is important for parallel configuration init/set/free and may be set within empty envelope instances. Therefore, it cannot be pushed down into Analyzer/Minimizer derived classes.

Referenced by DDACEDesignCompExp::DDACEDesignCompExp(), SurrBasedMinimizer::derived_free_communicators(), NonDGlobalReliability::derived_free_communicators(), NonDLocalInterval::derived_free_communicators(), NonDExpansion::derived_free_communicators(), NonDGlobalInterval::derived_free_communicators(), NonDGImpSampling::derived_free_communicators(), NonDAdaptiveSampling::derived_free_communicators(), NonDLocalReliability::derived_free_communicators(), NonDPolynomialChaos::derived_free_communicators(), Iterator::derived_free_communicators(), NonDBayesCalibration::derived_free_communicators(), SurrBasedMinimizer::derived_init_communicators(), NonDLocalInterval::derived_init_communicators(), NonDExpansion::derived_init_communicators(), NonDGlobalInterval::derived_init_communicators(), NonDGImpSampling::derived_init_communicators(), NonDAdaptiveSampling::derived_init_communicators(), NonDLocalReliability::derived_init_communicators(), NonDPolynomialChaos::derived_init_communicators(), NonDBayesCalibration::derived_init_communicators(), Iterator::derived_init_communicators(), SurrBasedMinimizer::derived_set_communicators(), NonDExpansion::derived_set_communicators(), NonDLocalReliability::derived_set_communicators(), NonDExpansion::derived_set_communicators(), NonDGlobalInterval::derived_set_communicators(), NonDGImpSampling::derived_set_communicators(), NonDAdaptiveSampling::derived_set_communicators(), NonDLocalReliability::derived_set_communicators(), NonDPolynomialChaos::derived_set_communicators(), NonDBayesCalibration::derived_set_communicators(), Iterator::derived_set_communicators(), NonD::derived_set_communicators(), NonDBayesCalibration::EffGlobalMinimizer(), Iterator::estimate_partition_bounds(), FSUDesignCompExp::FSUDesignCompExp(), NonDCubature::initialize_random_grid(), NonDQuadature::initialize_random_grid(), NonDSParseGrid::initialize_random_grid(), NonDExpansion::initialize_u_space_model(), JEGAOptimizer::JEGAOptimizer(), Iterator::maximum_evaluation_concurrency(), NonDAdaptImpSampling::NonDAdaptImpSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDCubature::NonDCubature(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDLHSInterval::NonDLHSInterval(), NonDMultilevelSampling::NonDMultilevelSampling(), NonDPolynomialChaos::NonDPolynomialChaos(), NonDQuadature::NonDQuadature(), NonDSampling::NonDSampling(), NonDSParseGrid::NonDSParseGrid(), Analyzer::num_samples(), ParamStudy::ParamStudy(), PSUADEDesignCompExp::PSUADEDesignComp-
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Exp(), Iterator::resize_communicators(), RichExtrapVerification::RichExtrapVerification(), APPSOptimizer::set_-apps_parameters(), COLINOptimizer::set_solver_parameters(), SNLLOptimizer::SNLLOptimizer(), and Iterator::<update_from_model>.

The documentation for this class was generated from the following files:

- Dakotaltertator.hpp
- Dakotalterator.cpp

13.68 IteratorScheduler Class Reference

This class encapsulates scheduling operations for concurrent sub-iteration within an outer level context (e.g., meta-iteration, nested models).

Public Member Functions

- **IteratorScheduler** (ParallelLibrary &parallel_lib, bool peer_assign_jobs, int num_servers=0, int procs_per_iterator=0, short scheduling=DEFAULT_SCHEDULING)
  
  constructor

- **~IteratorScheduler** ()
  
  destructor

- void **construct_sub_iterator** (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model, const String &method_ptr, const String &method_name, const String &model_ptr)
  
  instantiate sub_iterator on the current rank if not already constructed

- IntIntPair **configure** (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model)
  
  performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

- IntIntPair **configure** (ProblemDescDB &problem_db, const String &method_string, Iterator &sub_iterator, Model &sub_model)
  
  performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

- IntIntPair **configure** (ProblemDescDB &problem_db, Iterator &sub_iterator)
  
  performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

- void **partition** (int max_iterator_concurrency, IntIntPair &ppi_pr)
  
  convenience function for initializing iterator communicators, setting parallel configuration attributes, and managing outputs and restart.

- void **init_iterator** (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model)
  
  invokes static version of this function with appropriate parallelism level

- void **init_iterator** (ProblemDescDB &problem_db, const String &method_string, Iterator &sub_iterator, Model &sub_model)
  
  invokes static version of this function with appropriate parallelism level

- void **set_iterator** (Iterator &sub_iterator)
  
  invokes static version of this function with appropriate parallelism level

- void **run_iterator** (Iterator &sub_iterator)
  
  invokes static version of this function with appropriate parallelism level

- void **free_iterator** (Iterator &sub_iterator)
  
  invokes static version of this function with appropriate parallelism level

- void **free_iterator_parallelism** ()
convenience function for deallocating the concurrent iterator parallelism level

- template<typename MetaType >
  void schedule_iterators (MetaType &meta_object, Iterator &sub_iterator)
  
  short convenience function for distributing control among master_dynamic_schedule_iterators(), serve_iterators(), and peer_static_schedule_iterators()

- template<typename MetaType >
  void master_dynamic_schedule_iterators (MetaType &meta_object)

  executed by the scheduler master to manage a dynamic schedule of iterator jobs among slave iterator servers

- void stop_iterator_servers ()

  executed by the scheduler master to terminate slave iterator servers

- template<typename MetaType >
  void serve_iterators (MetaType &meta_object, Iterator &sub_iterator)

  executed on the slave iterator servers to perform iterator jobs assigned by the scheduler master

- template<typename MetaType >
  void peer_static_schedule_iterators (MetaType &meta_object, Iterator &sub_iterator)

  executed on iterator peers to manage a static schedule of iterator jobs

- void update (ParConfigLIter pc_iter)

  update schedPCIter

- void update (size_t index)

  update miPLIndex as well as associated settings for concurrent iterator scheduling from the corresponding Parallel-Level

- void update (ParConfigLIter pc_iter, size_t index)

  invoke update(ParConfigLIter) and update(size_t) in sequence

- void iterator_message_lengths (int params_msg_len, int results_msg_len)

  update paramsMsgLen and resultsMsgLen

- bool lead_rank () const

  determines if current processor is rank 0 of the parent comm

### Static Public Member Functions

- static void init_iterator (ProblemDescDB &problem_db, Iterator &sub_iterator, ParLevLIter pl_iter)

  convenience function for allocation of an iterator and (parallel) initialization of its comms

- static void init_iterator (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model, Par-LevLIter pl_iter)

  convenience function for allocation of an iterator and (parallel) initialization of its comms

- static void init_iterator (ProblemDescDB &problem_db, const String &method_string, Iterator &sub_iterator, Model &sub_model, Par-LevLIter pl_iter)

  convenience function for lightweight allocation of an iterator and (parallel) initialization of its comms

- static void set_iterator (Iterator &sub_iterator, ParLevLIter pl_iter)

  convenience function for setting comms prior to running an iterator

- static void run_iterator (Iterator &sub_iterator, ParLevLIter pl_iter)

  Convenience function for invoking an iterator and managing parallelism. This version omits communicator reparation. Function must be public due to use by MINLPNode.

- static void free_iterator (Iterator &sub_iterator, ParLevLIter pl_iter)

  convenience function for deallocating comms after running an iterator
Public Attributes

- **ParallelLibrary & parallelLib**
  reference to the *ParallelLibrary* instance
- **int numIteratorJobs**
  number of iterator executions to schedule
- **int numIteratorServers**
  number of concurrent iterator partitions
- **int procsPerIterator**
  partition size request
- **int iteratorCommRank**
  processor rank in *iteratorComm*
- **int iteratorCommSize**
  number of processors in *iteratorComm*
- **int iteratorServerId**
  identifier for an iterator server
- **bool messagePass**
  flag for message passing among iterator servers
- **short iteratorScheduling**
  \{DEFAULT,MASTER,PEER\}_SCHEDULING
- **bool peerAssignJobs**
  flag indicating need for peer 1 to assign jobs < to peers 2-n
- **ParConfigIter schedPCIter**
  iterator for active parallel configuration
- **size_t miPLIndex**
  index of active parallel level (corresponding < to ParallelConfiguration::miPLIers) to use < for parallelLib send/recv

Private Attributes

- **int paramsMsgLen**
  length of MPI buffer for parameter input instance(s)
- **int resultsMsgLen**
  length of MPI buffer for results output instance(s)

13.68.1 Detailed Description

This class encapsulates scheduling operations for concurrent sub-iteration within an outer level context (e.g., meta-iteration, nested models).

In time, a Scheduler class hierarchy is envisioned, but for now, this class is not part of a hierarchy.
13.68.2 Constructor & Destructor Documentation

IteratorScheduler ( ParallelLibrary & parallel_lib, bool peer_assign_jobs, int num_servers = 0, int proc_per_iterator = 0, short scheduling = DEFAULT_SCHEDULING )

constructor
Current constructor parameters are the input specification components, which are requests subject to override by ParallelLibrary::init_iterator_communicators().

13.68.3 Member Function Documentation

void init_iterator ( ProblemDescDB & problem_db, Iterator & sub_iterator, ParLevLIter pl_iter ) [static]

convenience function for allocation of an iterator and (parallel) initialization of its comms
This is a convenience function for encapsulating the allocation of communicators prior to running an iterator.
References ProblemDescDB::get_iterator(), ProblemDescDB::get_model(), ProblemDescDB::get_ushort(), Model::init_comms_bcast_flag(), Iterator::init_communicators(), Iterator::is_null(), Model::is_null(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_name(), Model::serve_init_communicators(), and Model::stop_init_communicators().

Referenced by MetaIterator::allocate_by_name(), MetaIterator::allocate_by_pointer(), Environment::construct(), ConcurrentMetaIterator::derived_init_communicators(), NestedModel::derived_init_communicators(), and IteratorScheduler::init_iterator().

void init_iterator ( ProblemDescDB & problem_db, Iterator & sub_iterator, Model & sub_model, ParLevLIter pl_iter ) [static]

convenience function for allocation of an iterator and (parallel) initialization of its comms
This is a convenience function for encapsulating the allocation of communicators prior to running an iterator.
References ProblemDescDB::get_iterator(), ProblemDescDB::get_ushort(), Model::init_comms_bcast_flag(), Iterator::init_communicators(), Iterator::is_null(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_name(), Model::serve_init_communicators(), and Model::stop_init_communicators().

void init_iterator ( ProblemDescDB & problem_db, const String & method_string, Iterator & sub_iterator, Model & sub_model, ParLevLIter pl_iter ) [static]

convenience function for lightweight allocation of an iterator and (parallel) initialization of its comms
This is a convenience function for encapsulating the allocation of communicators prior to running an iterator.
References ProblemDescDB::get_iterator(), Model::init_comms_bcast_flag(), Iterator::init_communicators(), Iterator::is_null(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_string(), Model::serve_init_communicators(), and Model::stop_init_communicators().

void set_iterator ( Iterator & sub_iterator, ParLevLIter pl_iter ) [static]

convenience function for setting comms prior to running an iterator
This is a convenience function for encapsulating the deallocation of communicators after running an iterator.
References Iterator::derived_set_communicators(), and Iterator::set_communicators().

Referenced by CollabHybridMetaIterator::derived_set_communicators(), EmbedHybridMetaIterator::derived_set_communicators(), ConcurrentMetaIterator::derived_set_communicators(), SeqHybridMetaIterator::derived_set_communicators(), NestedModel::derived_set_communicators(), and IteratorScheduler::set_iterator().
void run_iterator ( Iterator & sub_iterator, ParLevLIter pl_iter ) [static]

Convenience function for invoking an iterator and managing parallelism. This version omits communicator repartitioning. Function must be public due to use by MINLPNode.

This is a convenience function for encapsulating the parallel features (run/serve) of running an iterator. This function omits allocation/deallocation of communicators to provide greater efficiency in approaches that involve multiple iterator executions but only require communicator allocation/deallocation to be performed once.

References Model::finalize_mapping(), Model::initialize_mapping(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_name(), Iterator::resize(), Iterator::resize_communicators(), Iterator::run(), Model::serve_finalize_mapping(), Model::serve_init_mapping(), Model::serve_run(), Model::stop_finalize_mapping(), Model::stop_init_mapping(), and Model::stop_servers().

Referenced by NestedModel::derived_evaluate(), Environment::execute(), IteratorScheduler::peer_static_schedule_iterators(), IteratorScheduler::run_iterator(), and IteratorScheduler::serve_iterators().

void free_iterator ( Iterator & sub_iterator, ParLevLIter pl_iter ) [static]

Convenience function for deallocating comms after running an iterator.

This is a convenience function for encapsulating the deallocation of communicators after running an iterator.

References Iterator::derived_free_communicators(), Iterator::free_communicators(), and Iterator::method_name().

Referenced by CollabHybridMetaIterator::derived_free_communicators(), EmbedHybridMetaIterator::derived_free_communicators(), ConcurrentMetaIterator::derived_free_communicators(), SeqHybridMetaIterator::derived_free_communicators(), NestedModel::derived_free_communicators(), Environment::destruct(), and IteratorScheduler::free_iterator().

IntIntPair configure ( ProblemDescDB & problem_db, Iterator & sub_iterator, Model & sub_model )

performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

This is a convenience function for computing the minimum and maximum partition size prior to concurrent iterator partitioning.

References ProblemDescDB::get_iterator(), IteratorScheduler::schedPCIter, and ParallelLevel::server_communicator_rank().

Referenced by IteratorScheduler::configure(), ConcurrentMetaIterator::derived_init_communicators(), NestedModel::derived_init_communicators(), MetaIterator::estimate_by_name(), and MetaIterator::estimate_by_pointer().

IntIntPair configure ( ProblemDescDB & problem_db, const String & method_string, Iterator & sub_iterator, Model & sub_model )

performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

This is a convenience function for computing the minimum and maximum partition size prior to concurrent iterator partitioning.

References IteratorScheduler::configure(), ProblemDescDB::get_iterator(), IteratorScheduler::schedPCIter, and ParallelLevel::server_communicator_rank().

IntIntPair configure ( ProblemDescDB & problem_db, Iterator & sub_iterator )

performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

This is a convenience function for computing the minimum and maximum partition size prior to concurrent iterator partitioning.

References ParallelLibrary::bcast(), Iterator::estimate_partition_bounds(), ProblemDescDB::get_db_method_node(), ProblemDescDB::get_db_model_node(), IteratorScheduler::parallelLib, IteratorScheduler::schedPCIter,
void partition ( int max_iterator_concurrency, IntIntPair & ppi )

Convenience function for initializing iterator communicators, setting parallel configuration attributes, and managing outputs and restart.

Called from derived class constructors once maxIteratorConcurrency is defined but prior to instantiating Iterators and Models.

References ParallelLibrary::init_iterator_communicators(), IteratorScheduler::iteratorScheduling, IteratorScheduler::numIteratorServers, ParallelLibrary::parallel_configuration_iterator(), IteratorScheduler::parallelLib, IteratorScheduler::procsPerIterator, ParallelLibrary::push_output_tag(), and IteratorScheduler::update().

Referenced by CollabHybridMetaIterator::derived_initCommunicators(), EmbedHybridMetaIterator::derived_initCommunicators(), ConcurrentMetaIterator::derived_initCommunicators(), SeqHybridMetaIterator::derived_initCommunicators(), and NestedModel::derived_initCommunicators().

void schedule_iterators ( MetaType & meta_object, Iterator & sub_iterator )

Short convenience function for distributing control among master_dynamic_schedule_iterators(), serve_iterators(), and peer_static_schedule_iterators()

This implementation supports the scheduling of multiple jobs using a single iterator/model pair. Additional (overloaded) implementations could involve independent iterator instances.

References IteratorScheduler::iteratorScheduling, IteratorScheduler::iteratorServerId, IteratorScheduler::lead_rank(), IteratorScheduler::master_dynamic_schedule_iterators(), IteratorScheduler::numIteratorServers, ParallelLibrary::parallel_configuration_iterator(), IteratorScheduler::parallelLib, IteratorScheduler::peer_static_schedule_iterators(), IteratorScheduler::serve_iterators(), and IteratorScheduler::stop_iterator_servers().

Referenced by CollabHybridMetaIterator::core_run(), EmbedHybridMetaIterator::core_run(), ConcurrentMetaIterator::core_run(), NestedModel::derived_synchronize(), SeqHybridMetaIterator::run_sequential(), and NestedModel::serve_run().

void master_dynamic_schedule_iterators ( MetaType & meta_object )

Executed by the scheduler master to manage a dynamic schedule of iterator jobs among slave iterator servers

This function is adapted from ApplicationInterface::master_dynamic_schedule_evaluations().

References ParallelLibrary::free(), ParallelLibrary::irecv_mi(), ParallelLibrary::isend_mi(), IteratorScheduler::miPLIndex, IteratorScheduler::numIteratorJobs, IteratorScheduler::numIteratorServers, IteratorScheduler::parallelLib, MPIPackBuffer::reset(), MPIUnpackBuffer::resize(), IteratorScheduler::resultsMsgLen, ParallelLibrary::waitall(), and ParallelLibrary::waitsome().

Referenced by IteratorScheduler::serve_iterators().

void serve_iterators ( MetaType & meta_object, Iterator & sub_iterator )

Executed on the slave iterator servers to perform iterator jobs assigned by the scheduler master

This function is similar in structure to ApplicationInterface::serve_evaluations_synth().

References ParallelLibrary::bcast_i(), IteratorScheduler::iteratorCommRank, IteratorScheduler::iteratorCommSize, IteratorScheduler::miPLIndex, ParallelLibrary::parallel_time(), IteratorScheduler::parallelLib, IteratorScheduler::paramsMsgLen, ParallelLibrary::recv_mi(), IteratorScheduler::resultsMsgLen, IteratorScheduler::run_iterator(), and ParallelLibrary::send_mi().

Referenced by IteratorScheduler::schedule_iterators().

The documentation for this class was generated from the following files:
13.69 JEGAOptimizer Class Reference

A version of Dakota::Optimizer for instantiation of John Eddy’s Genetic Algorithms (JEGA).

Inheritance diagram for JEGAOptimizer:

Classes

- class Driver
  
  A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.

- class Evaluator

  An evaluator specialization that knows how to interact with Dakota.

- class EvaluatorCreator

  A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.

Public Member Functions

- virtual void core_run ()
  
  Performs the iterations to determine the optimal set of solutions.

- virtual bool accepts_multiple_points () const

  Overridden to return true since JEGA algorithms can accept multiple initial points.

- virtual bool returns_multiple_points () const

  Overridden to return true since JEGA algorithms can return multiple final points.

- virtual void initial_points (const VariablesArray &pts)

  Overridden to assign the _initPts member variable to the passed in collection of Dakota::Variables.

- virtual const VariablesArray & initial_points () const

  Overridden to return the collection of initial points for the JEGA algorithm created and run by this JEGAOptimizer.

- JEGAOptimizer (ProblemDescDB &problem_db, Model &model)

  Constructs a JEGAOptimizer class object.

- ~JEGAOptimizer ()

  Destructs a JEGAOptimizer.
Protected Member Functions

- void `LoadDakotaResponses` (const JEGA::Utilities::Design &from, Variables &vars, Response &resp) const
  
  Loads the JEGA-style Design class into equivalent Dakota-style Variables and Response objects.

- void `ReCreateTheParameterDatabase`() 
  
  Destroys the current parameter database and creates a new empty one.

- void `LoadTheParameterDatabase` ()
  
  Reads information out of the known Dakota::ProblemDescDB and puts it into the current parameter database.

- void `LoadAlgorithmConfig` (JEGA::FrontEnd::AlgorithmConfig &aConfig)
  
  Completely initializes the supplied algorithm configuration.

- void `LoadProblemConfig` (JEGA::FrontEnd::ProblemConfig &pConfig)
  
  Completely initializes the supplied problem configuration.

- void `LoadTheDesignVariables` (JEGA::FrontEnd::ProblemConfig &pConfig)
  
  Adds DesignVariableInfo objects into the problem configuration object.

- void `LoadTheObjectiveFunctions` (JEGA::FrontEnd::ProblemConfig &pConfig)
  
  Adds ObjectiveFunctionInfo objects into the problem configuration object.

- void `LoadTheConstraints` (JEGA::FrontEnd::ProblemConfig &pConfig)
  
  Adds ConstraintInfo objects into the problem configuration object.

- void `GetBestSolutions` (const JEGA::Utilities::DesignOFSortSet &from, const JEGA::Algorithms::GeneticAlgorithm &theGA, std::multimap<RealRealPair, JEGA::Utilities::Design *> &designSortMap)
  
  Returns up to `numBest` designs sorted by DAKOTA’s fitness (L2 constraint violation, then utopia or objective),
  taking into account the algorithm type. The front of the returned map can be viewed as a single “best”.

- void `GetBestMOSolutions` (const JEGA::Utilities::DesignOFSortSet &from, const JEGA::Algorithms::GeneticAlgorithm &theGA, std::multimap<RealRealPair, JEGA::Utilities::Design *> &designSortMap)
  
  Retrieve the best Designs from a set of solutions assuming that they are generated by a multi objective algorithm.

- void `GetBestSOSolutions` (const JEGA::Utilities::DesignOFSortSet &from, const JEGA::Algorithms::GeneticAlgorithm &theGA, std::multimap<RealRealPair, JEGA::Utilities::Design *> &designSortMap)
  
  Retrieve the best Designs from a set of solutions assuming that they are generated by a single objective algorithm.

- JEGA::DoubleMatrix `ToDoubleMatrix` (const VariablesArray &variables) const
  
  Converts the items in a VariablesArray into a DoubleMatrix whereby the items in the matrix are the design variables.

Private Attributes

- EvaluatorCreator * _theEvalCreator
  
  A pointer to an EvaluatorCreator used to create the evaluator used by JEGA in Dakota (a JEGAEvaluator).

- JEGA::Utilities::ParameterDatabase * _theParamDB
  
  A pointer to the ParameterDatabase from which all parameters are retrieved by the created algorithms.

- VariablesArray _initPts
  
  An array of initial points to use as an initial population.

Additional Inherited Members

13.69.1 Detailed Description

A version of Dakota::Optimizer for instantiation of John Eddy’s Genetic Algorithms (JEGA).

This class encapsulates the necessary functionality for creating and properly initializing the JEGA algorithms
(MOGA and SOGA).
13.69.2 Constructor & Destructor Documentation

**JEGAOptimizer ( ProblemDescDB & problem_db, Model & model )**

Constructs a JEGAOptimizer class object.

This method does some of the initialization work for the algorithm. In particular, it initialized the JEGA core.

**Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>problem_db</code></td>
<td>The Dakota::ProblemDescDB with information on how the algorithm controls should be set.</td>
</tr>
<tr>
<td><code>model</code></td>
<td>The Dakota::Model that will be used by this optimizer for problem information, etc.</td>
</tr>
</tbody>
</table>

References JEGAOptimizer::theEvalCreator, ProblemDescDB::get_int(), ProblemDescDB::get_short(), Iterator::iteratedModel, JEGAOptimizer::LoadTheParameterDatabase(), Iterator::maxEvalConcurrency, Iterator::methodName, Iterator::numFinalSolutions, and Iterator::probDescDB.

13.69.3 Member Function Documentation

**void LoadDakotaResponses ( const JEGA::Utilities::Design & from, Dakota::Variables & vars, Dakota::Response & resp ) const** [protected]

Loads the JEGA-style Design class into equivalent Dakota-style Variables and Response objects.

This version is meant for the case where a Variables and a Response object exist and just need to be loaded.

**Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>from</code></td>
<td>The JEGA Design class object from which to extract the variable and response information for Dakota.</td>
</tr>
<tr>
<td><code>vars</code></td>
<td>The Dakota::Variables object into which to load the design variable values of <code>from</code>.</td>
</tr>
<tr>
<td><code>resp</code></td>
<td>The Dakota::Response object into which to load the objective function and constraint values of <code>from</code>.</td>
</tr>
</tbody>
</table>

References Variables::continuous_variables(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), Variables::discrete_string_variable(), Response::function_values(), and Dakota::set_index_to_value().

**void LoadTheParameterDatabase ( )** [protected]

Reads information out of the known Dakota::ProblemDescDB and puts it into the current parameter database.

This should be called from the JEGAOptimizer constructor since it is the only time when the problem description database is certain to be configured to supply data for this optimizer.

Referenced by JEGAOptimizer::JEGAOptimizer().

**void LoadAlgorithmConfig ( JEGA::FrontEnd::AlgorithmConfig & aConfig )** [protected]

Completely initializes the supplied algorithm configuration.

This loads the supplied configuration object with appropriate data retrieved from the parameter database.

**Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>aConfig</code></td>
<td>The algorithm configuration object to load.</td>
</tr>
</tbody>
</table>

**void LoadProblemConfig ( JEGA::FrontEnd::ProblemConfig & pConfig )** [protected]

Completely initializes the supplied problem configuration.
This loads the fresh configuration object using the LoadTheDesignVariables, LoadTheObjectiveFunctions, and LoadTheConstraints methods.
Parameters

\begin{tabular}{|l|l|}
\hline
\textit{pConfig} & The problem configuration object to load. \\
\hline
\end{tabular}

\begin{verbatim}
void LoadTheDesignVariables ( JEGA::FrontEnd::ProblemConfig & pConfig ) [protected]

Adds DesignVariableInfo objects into the problem configuration object.
This retrieves design variable information from the ParameterDatabase and creates DesignVariableInfo’s from it.
Parameters

\begin{tabular}{|l|l|}
\hline
\textit{pConfig} & The problem configuration object to load. \\
\hline
\end{tabular}

References Model::continuous_lower_bounds().
\end{verbatim}

\begin{verbatim}
void LoadTheObjectiveFunctions ( JEGA::FrontEnd::ProblemConfig & pConfig ) [protected]

Adds ObjectiveFunctionInfo objects into the problem configuration object.
This retrieves objective function information from the ParameterDatabase and creates ObjectiveFunctionInfo’s from it.
Parameters

\begin{tabular}{|l|l|}
\hline
\textit{pConfig} & The problem configuration object to load. \\
\hline
\end{tabular}

\end{verbatim}

\begin{verbatim}
void LoadTheConstraints ( JEGA::FrontEnd::ProblemConfig & pConfig ) [protected]

Adds ConstraintInfo objects into the problem configuration object.
This retrieves constraint function information from the ParameterDatabase and creates ConstraintInfo’s from it.
Parameters

\begin{tabular}{|l|l|}
\hline
\textit{pConfig} & The problem configuration object to load. \\
\hline
\end{tabular}

References Dakota::asstring(), Dakota::copy_row_vector(), and Model::nonlinear_ineq_constraint_lower_bounds().
\end{verbatim}

\begin{verbatim}
void GetBestSolutions ( const JEGA::Utilities::DesignOFSortSet & from, const JEGA::Algorithms::GeneticAlgorithm & theGA, std::multimap< RealRealPair, JEGA::Utilities::Design * > & designSortMap ) [protected]

Returns up to _numBest designs sorted by DAKOTA’s fitness (L2 constraint violation, then utopia or objective), taking into account the algorithm type. The front of the returned map can be viewed as a single "best".
Parameters

\begin{tabular}{|l|l|}
\hline
\textit{from} & The full set of designs returned by the solver. \\
\hline
\textit{theGA} & The GA used to generate this set; needed for its weights in the SO case, provided to both for consistency \\
\hline
\textit{designSortMap} & Map of best solutions with key pair<constraintViolation, fitness> \\
\hline
\end{tabular}

eventually this functionality must be moved into a separate post-processing application for MO datasets.
\end{verbatim}
void GetBestMOSolutions ( const JEGA::Utilities::DesignOFSortSet & from, const JEGA::Algorithms::GeneticAlgorithm & theGA, std::multimap<RealRealPair, JEGA::Utilities::Design *> & designSortMap ) [protected]
Retreive the best Designs from a set of solutions assuming that they are generated by a multi objective algorithm. eventually this functionality must be moved into a separate post-processing application for MO datasets.

void GetBestSOSolutions ( const JEGA::Utilities::DesignOFSortSet & from, const JEGA::Algorithms::GeneticAlgorithm & theGA, std::multimap<RealRealPair, JEGA::Utilities::Design *> & designSortMap ) [protected]
Retreive the best Designs from a set of solutions assuming that they are generated by a single objective algorithm. eventually this functionality must be moved into a separate post-processing application for MO datasets.
References Dakota::abort_handler().

JEGA::DoubleMatrix ToDoubleMatrix ( const VariablesArray & variables ) const [protected]
Converts the items in a VariablesArray into a DoubleMatrix whereby the items in the matrix are the design variables.
The matrix will not contain responses but when being used by Dakota, this doesn’t matter. JEGA will attempt to re-evaluate these points but Dakota will recognize that they do not require re-evaluation and thus it will be a cheap operation.
Parameters

| variables | The array of DakotaVariables objects to use as the contents of the returned matrix. |

Returns
The matrix created using the supplied VariablesArray.

void core_run ( ) [virtual]
Performs the iterations to determine the optimal set of solutions.
Override of pure virtual method in Optimizer base class.
The extraction of parameter values actually occurs in this method when the JEGA::FrontEnd::Driver::ExecuteAlgorithm is called. Also the loading of the problem and algorithm configurations occurs in this method. That way, if it is called more than once and the algorithm or problem has changed, it will be accounted for.
Reimplemented from Iterator.
References JEGAOptimizer::Driver::DestroyAlgorithm(), JEGAOptimizer::Driver::ExtractAllData(), and JEGA::FrontEnd::Driver::PerformIterations().

bool accepts_multiple_points ( ) const [virtual]
Overridden to return true since JEGA algorithms can accept multiple initial points.
Returns
true, always.
Reimplemented from Iterator.
bool returns_multiple_points() const [virtual]
Overridden to return true since JEGA algorithms can return multiple final points.
Returns
true, always.
Reimplemented from Iterator.

void initial_points(const VariablesArray &pts) [virtual]
Overridden to assign the _initPts member variable to the passed in collection of Dakota::Variables.
Parameters
| pts | The array of initial points for the JEGA algorithm created and run by this JEGAOptimizer.
Reimplemented from Iterator.

const VariablesArray & initial_points() const [virtual]
Overridden to return the collection of initial points for the JEGA algorithm created and run by this JEGA-Optimizer.
Returns
The collection of initial points for the JEGA algorithm created and run by this JEGAOptimizer.
Reimplemented from Iterator.

13.69.4 Member Data Documentation

VariablesArray _initPts [private]
An array of initial points to use as an initial population.
This member is here to help support the use of JEGA algorithms in Dakota strategies. If this array is populated, then whatever initializer is specified will be ignored and the DoubleMatrix initializer will be used instead on a matrix created from the data in this array.
The documentation for this class was generated from the following files:

- JEGAOptimizer.hpp
- JEGAOptimizer.cpp

13.70 LabelsWriter Class Reference
Utility used in derived write_core to write labels in tabular format.

Public Member Functions

- template<typename ArrayType>
  void operator() (std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array)
13.70.1 Detailed Description

Utility used in derived write_core to write labels in tabular format.

13.70.2 Member Function Documentation

```cpp
void operator() ( std::ostream & s, size_t start_index, size_t num_items, const ArrayType & array_data, StringMultiArrayConstView label_array ) [inline]
```

The tabular labels writer only forwards the label arrays.

The documentation for this class was generated from the following file:

- DakotaVariables.hpp

13.71 LeastSq Class Reference

Base class for the nonlinear least squares branch of the iterator hierarchy.

Inheritance diagram for LeastSq:

```
LeastSq
   |   
   v   
Minimizer
   |   
   v   
Iterator
   |   
   v   
LeastSq
     |   
     v
NL2SOLLeastSq
     |   
     v
NLSSOLLeastSq
     |   
     v
SNLLLeastSq
```

Protected Member Functions

- LeastSq ()
  default constructor
- LeastSq (ProblemDescDB &problem_db, Model &model)
  standard constructor
- LeastSq (unsigned short method_name, Model &model)
  alternate "on the fly" constructor
- ~LeastSq ()
  destructor
- void initialize_run ()
- void post_run (std::ostream &s)
- void finalize_run ()
  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- void print_results (std::ostream &s)
- void get_confidence_intervals ()
  Calculate confidence intervals on estimated parameters.
CHAPTER 13. CLASS DOCUMENTATION

Protected Attributes

- `size_t numLeastSqTerms`  
  number of least squares terms
- `LeastSq * prevLSqInstance`  
  pointer containing previous value of leastSqInstance
- `bool weightFlag`  
  flag indicating whether weighted least squares is active
- `RealVector confBoundsLower`  
  lower bounds for confidence intervals on calibration parameters
- `RealVector confBoundsUpper`  
  upper bounds for confidence intervals on calibration parameters

Static Protected Attributes

- `static LeastSq * leastSqInstance`  
  pointer to LeastSq instance used in static member functions

Private Member Functions

- `void weight_model ()`  
  Wrap iteratedModel in a RecastModel that weights the residuals.

Static Private Member Functions

- `static void primary_resp_weighter (const Variables &unweighted_vars, const Variables &weighted_vars, const Response &unweighted_response, Response &weighted_response)`  
  Recast callback function to weight least squares residuals, gradients, and Hessians.

Additional Inherited Members

13.71.1 Detailed Description

Base class for the nonlinear least squares branch of the iterator hierarchy.

The LeastSq class provides common data and functionality for least squares solvers (including NL2OL, NLSSOLLeastSq, and SNLLLeastSq.

13.71.2 Constructor & Destructor Documentation

LeastSq (`ProblemDescDB & problem_db, Model & model`) [protected]

standard constructor

This constructor extracts the inherited data for the least squares branch and performs sanity checking on gradient and constraint settings.

References Dakota::abort_handler(), Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, Variables::copy(), Model::current_variables(), Minimizer::data_transform_model(), Iterator::iteratedModel, Iterator::method_Name, LeastSq::numLeastSqTerms, Minimizer::numTotalCalibTerms, Minimizer::optimizationFlag, Model::primary_fn_type(), Minimizer::scale_model(), Minimizer::scaleFlag, LeastSq::weight_model(), and LeastSq::weightFlag.
13.71. LEASTSQ CLASS REFERENCE

13.71.3 Member Function Documentation

void initialize_run( ) [protected], [virtual]

This function should be invoked (or reimplemented) by any derived implementations of initialize_run() (which would otherwise hide it).

- Reimplemented from Iterator.
- Reimplemented in SNLLLeastSq.
- References Minimizer::initialize_run(), Iterator::iteratedModel, LeastSq::leastSqInstance, Iterator::myModel-Layers, LeastSq::prevLSqInstance, and Model::update_from_subordinate_model().
- Referenced by SNLLLeastSq::initialize_run().

void post_run ( std::ostream & s ) [protected], [virtual]

Implements portions of post_run specific to LeastSq for scaling back to native variables and functions. This function should be invoked (or reimplemented) by any derived implementations of post_run() (which would otherwise hide it) transform variables back to inbound model, before any potential lookup

- Reimplemented from Iterator.
- Reimplemented in SNLLLeastSq.
- References Dakota::abort_handler(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, Variables::continuous_variables(), ScalingModel::cv_scaled2native(), Minimizer::expData, Response::function_value(), Response::function_values(), Response::function_values_view(), LeastSq::get_confidence_intervals(), ExperimentData::interpolate_flag(), Iterator::iteratedModel, Minimizer::local_recast_retrieve(), Model::model_rep(), LeastSq::numLeastSqTerms, Minimizer::numUserPrimaryFns, Minimizer::post_run(), Model::primary_response_fn_weights(), ExperimentData::recover_model(), ScalingModel::resp_scaled2native(), Minimizer::scalingModel, Model::subordinate_model(), and LeastSq::weightFlag.

void finalize_run ( ) [inline], [protected], [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

- Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s finalize_run(), typically after performing its own implementation steps.
- Reimplemented from Iterator.
- Reimplemented in SNLLLeastSq.
- References Minimizer::finalize_run(), LeastSq::leastSqInstance, and LeastSq::prevLSqInstance.
- Referenced by SNLLLeastSq::finalize_run().

void print_results ( std::ostream & s ) [protected], [virtual]

Redefines default iterator results printing to include nonlinear least squares results (residual terms and constraints).

- Reimplemented from Iterator.
- References Iterator::activeSet, Minimizer::archive_allocate_best(), Minimizer::archive_best(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, LeastSq::confBoundsLower, LeastSq::confBoundsUpper, ExperimentData::config_vars(), Model::continuous_variable_labels(), Dakota::data_pairs, Minimizer::dataTransformModel, Minimizer::expData, Model::interface_id(), Iterator::iteratedModel, Dakota::lookup_by_val(), Model::model_rep(), ExperimentData::num_experiments(), Model::num_functions(), Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, Minimizer::original_model(), Model::primary_response_fn_weights(), DataTransformModel::print_best_responses(), Minimizer::print_residuals(), ActiveSet::request_values(), Model::subordinate_model(), and Dakota::write_precision.
void get_confidence_intervals() [protected]

Calculate confidence intervals on estimated parameters.

Calculate individual confidence intervals for each parameter. These bounds are based on a linear approximation of the nonlinear model.

References Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, LeastSq::confBoundsLower, LeastSq::confBoundsUpper, Model::continuous_variables(), Response::copy(), Model::current_response(), DataTransformModel::data_transform_response(), Minimizer::dataTransformModel, Model::evaluate(), Response::function_gradients(), Iterator::iteratedModel, Model::model_rep(), Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, ActiveSet::request_values(), Minimizer::scaleFlag, and Minimizer::vendorNumericalGradFlag.

Referenced by LeastSq::post_run(), and SNLLLeastSq::post_run().

void weight_model() [private]

Wrap iteratedModel in a RecastModel that weights the residuals.

Setup Recast for weighting model. The weighting transformation doesn’t resize, so use numUserPrimaryFns. No vars, active set or secondary mapping. All indices are one-to-one mapped (no change in counts).

References Model::assign_rep(), Model::current_response(), Response::function_gradients(), Response::function_hessians(), Iterator::iteratedModel, Iterator::myModelLayers, Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, Minimizer::numNonlinearConstraints, Minimizer::numNonlinearIneqConstraints, Iterator::outputLevel, LeastSq::primaryResp_weighter(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), and Model::subordinate_model().

Referenced by LeastSq::LeastSq().

void primary_resp_weighter(const Variables & unweighted_vars, const Variables & weighted_vars, const Response & unweighted_response, Response & weighted_response) [static], [private]

Recast callback function to weight least squares residuals, gradients, and Hessians.

Apply weights to least squares residuals

References Dakota::NPOS, Response::active_set_derivative_vector(), Response::active_set_request_vector(), Variables::acv(), Variables::all_continuous_variable_ids(), Variables::continuous_variable_ids(), Variables::cv(), Dakota::find_index(), Response::function_gradients(), Response::function_gradients_view(), Response::function_hessian(), Response::function_hessian_view(), Response::function_values(), Response::function_values_view(), Variables::icv(), Variables::inactive_continuous_variable_ids(), Iterator::iteratedModel, LeastSq::leastSqInstance, LeastSq::numLeastSqTerms, Iterator::outputLevel, Model::primary_response_fn_weights(), and Model::subordinate_model().

Referenced by LeastSq::weight_model().

The documentation for this class was generated from the following files:

- DakotaLeastSq.hpp
- DakotaLeastSq.cpp

13.72 LibraryEnvironment Class Reference

Environment corresponding to execution as an embedded library.

Inheritance diagram for LibraryEnvironment:
Public Member Functions

- **LibraryEnvironment ()**
  *default constructor*

- **LibraryEnvironment (ProgramOptions prog_opts, bool check_bcast_construct=true, DbCallbackFunctionPtr callback=NULL, void *callback_data=NULL)*
  Primary constructor: program options typically specifies an input file or input string. Optionally specify a callback function to be invoked after parsing. Set check_bcast_construct if performing late updates and later calling `done_modifying_db()`.

- **LibraryEnvironment (MPI_Comm dakota_mpi_comm, ProgramOptions prog_opts=ProgramOptions(), bool check_bcast_construct=true, DbCallbackFunctionPtr callback=NULL, void *callback_data=NULL)*
  Alternate constructor accepting communicator, same options as primary.

- **~LibraryEnvironment ()**
  *destructor*

- **void insert_nodes (Dakota::DataMethod &dme, Dakota::DataModel &dmo, Dakota::DataVariables &dv, Dakota::DataInterface &di, Dakota::DataResponses &dr)*
  Insert DB nodes for a `{Method,Model,Variables,Interface,Responses}` set.

- **void done_modifying_db ()**
  Check database contents, broadcast, and construct iterators.

- **bool plugin_interface (const String &model_type, const String &interf_type, const String &an_driver, Interface *plugin_iface)*
  Plug-in the passed interface into any interface matching the specified (possibly empty) model, interface, and driver strings; returns true if a plugin was performed.

- **InterfaceList filtered_interface_list (const String &interf_type, const String &an_driver)*
  filter the available `Interface` instances based on matching interface type and analysis drivers (empty String matches any)

- **ModelList filtered_model_list (const String &model_type, const String &interf_type, const String &an_-driver)*
  filter the available `Model` instances based on matching model type, interface type, and analysis drivers (empty String matches any)

Additional Inherited Members

### 13.72.1 Detailed Description

**Environment** corresponding to execution as an embedded library.

This environment corresponds to use of Dakota as a library within another application, e.g., within `library_mode.cpp`. It sets up the `ParallelLibrary` and `ProblemDescDB` objects without access to command line arguments.
13.72.2 Constructor & Destructor Documentation

LibraryEnvironment ( ProgramOptions prog_opts, bool check_bcast_construct = true,
DbCallbackFunctionPtr callback = NULL, void * callback_data = NULL )

Primary constructor: program options typically specifies an input file or input string. Optionally specify a callback
function to be invoked after parsing. Set check_bcast_construct if performing late updates and later calling done_modifying_db().

Construct library environment, optionally performing check/bcast of database and iterator construction

References Environment::construct(), OutputManager::output_startup_message(), Environment::outputManager, and Environment::parse().

LibraryEnvironment ( MPI_Comm dakota_mpi_comm, ProgramOptions prog_opts = ProgramOptions(),
bool check_bcast_construct = true, DbCallbackFunctionPtr callback = NULL, void * callback_data = NULL )

Alternate constructor accepting communicator, same options as primary.

Construct library environment on passed MPI Comm, optionally performing check/bcast of database and
iterator construction. MPI Comm is first argument so client doesn’t have to pass all args

References Environment::construct(), OutputManager::output_startup_message(), Environment::outputManager, and Environment::parse().

13.72.3 Member Function Documentation

InterfaceList filtered_interface_list ( const String & interf_type, const String & an_driver )

filter the available Interface instances based on matching interface type and analysis drivers (empty String matches any)

This convenience function helps clients locate and plugin to the right Interface instance for simple cases. Pass
an empty string to match any instead of a specific instance

References Interface::analysis_drivers(), Dakota::contains(), Interface::interface_type(), ProblemDescDB::model_list(), and Environment::probDescDB.

ModelList filtered_model_list ( const String & model_type, const String & interf_type, const String & an_driver )

filter the available Model instances based on matching model type, interface type, and analysis drivers (empty String matches any)

This convenience function helps clients locate and plugin to the right Interface instance for cases where the
parallel configuration is needed in constructing a parallel plugin. Pass an empty string to match any instead of a
specific instance

References Interface::analysis_drivers(), Dakota::contains(), Interface::interface_type(), ProblemDescDB::model_list(), and Environment::probDescDB.

Referenced by parallel_interface_plugin(), LibraryEnvironment::plugin_interface(), run_dakota(), and run_dakota_mixed().

The documentation for this class was generated from the following files:

- LibraryEnvironment.hpp
- LibraryEnvironment.cpp
13.73 LightWtBaseConstructor Struct Reference

Dummy struct for overloading constructors used in on-the-fly Model instantiations.

Public Member Functions

- LightWtBaseConstructor (int=0)
  
  C++ structs can have constructors.

13.73.1 Detailed Description

Dummy struct for overloading constructors used in on-the-fly Model instantiations.

LightWtBaseConstructor is used to overload the constructor used for on-the-fly Model instantiations. Putting this struct here avoids circular dependencies.

The documentation for this struct was generated from the following file:

- dakota.global_defs.hpp

13.74 MatchesWC Struct Reference

Predicate that returns true when the passed path matches the wildcard with which it was configured. Currently supports * and ?.

Public Member Functions

- MatchesWC (const bfs::path &wild_card)
  
  ctor that builds and stores the regular expression

- bool operator() (const bfs::path &dir_entry)
  
  return true is dir_entry matches wildCardRegEx

Public Attributes

- boost::basic_regex
  
  < bfs::path::value_type > wildCardRegEx
  
  archived RegEx; wchar-based on Windows

13.74.1 Detailed Description

Predicate that returns true when the passed path matches the wildcard with which it was configured. Currently supports * and ?.

The documentation for this struct was generated from the following file:

- WorkdirHelper.hpp
13.75 MatlabInterface Class Reference

Inheritance diagram for MatlabInterface:

```
Interface
  ApplicationInterface
    DirectApplicInterface
      MatlabInterface
```

**Public Member Functions**

- `MatlabInterface (const ProblemDescDB &problem_db)`  
  Constructor: start Matlab engine.
- `~MatlabInterface ()`  
  Destructor: close Matlab engine.

**Protected Member Functions**

- `virtual int derived_map_ac (const String &ac_name)`  
  execute an analysis code portion of a direct evaluation invocation
- `int matlab_engine_run (const Dakota::String &ac_name)`  
  Helper function supporting derived_map_ac. Sends data to Matlab, executes analysis, collects return data.
- `int matlab_field_prep (mxArray *dakota_matlab, const char *field_name)`  
  check that the dakota_matlab strucutre has the specified field_name and add if necessary; free structure memory in preparation for new alloc

**Protected Attributes**

- `engine * matlabEngine`  
  pointer to the MATLAB engine used for direct evaluations

13.75.1 Detailed Description

Specialization of DirectApplicInterface to link to Matlab analysis drivers. Includes convenience functions to map data to/from Matlab

13.75.2 Member Function Documentation

`int derived_map_ac ( const String & ac_name ) [protected], [virtual]`

execute an analysis code portion of a direct evaluation invocation  
Matlab specialization of dervied analysis components.
Reimplemented from DirectApplicInterface. References ApplicationInterface::analysisServerId, and MatlabInterface::matlab_engine_run().

```cpp
int matlab_engine_run ( const Dakota::String & ac_name ) [protected]
```

Helper function supporting derived_map_ac. Sends data to Matlab, executes analysis, collects return data.

Direct interface to Matlab through Mathworks external API. M-file executed is specified through analysis_drivers, extra strings through analysis_components. (Original BMA 11/28/2005)

Special thanks to Lee Peterson for substantial enhancements 12/15/2007: Added output buffer for the M-ATLAB command response and error messages Made the Dakota variable persistent in the MATLAB engine workspace Added robustness to the user deleting required Dakota fields

References Dakota::abort_handler(), DirectApplicInterface::analysisComponents, DirectApplicInterface::analysis-DriverIndex, Interface::currEvalId, DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, Dakota::FIELD_NAMES, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, Interface::fnLabels, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface::hessFlag, MatlabInterface::matlab_field_prep(), MatlabInterface::matlabEngine, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADIV, Dakota::NUMBER_OF_FIELDS, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, DirectApplicInterface::numVars, Interface::outputLevel, DirectApplicInterface-::xC, DirectApplicInterface::xCLabels, DirectApplicInterface::xDI, DirectApplicInterface::xDILabels, DirectApplicInterface::xDR, and DirectApplicInterface::xDRLabels.

Referenced by MatlabInterface::derived_map_ac().

The documentation for this class was generated from the following files:

- MatlabInterface.hpp
- MatlabInterface.cpp

## 13.76 MetaIterator Class Reference

Base class for meta-iterators.

Inheritance diagram for MetaIterator:

```
+-------------------+          +-------------------+          +-------------------+
| Iterator           |          | MetaIterator       |          | MetaIterator       |
|                   |          |  CollabHybridMetaIterator |  ConcurrentMetaIterator |  EmbedHybridMetaIterator |  SeqHybridMetaIterator |
```

### Public Member Functions

- `bool resize ()`

  reinitializes iterator based on new variable size

### Protected Member Functions

- `MetaIterator (ProblemDescDB &problem_db)`

  standard constructor

- `MetaIterator (ProblemDescDB &problem_db, Model &model)`
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alternate constructor
• ∼MetaIterator ()

destructor
• void post_run (std::ostream &s)
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
• void check_model (const String &method_ptr, const String &model_ptr)
  check that a model identified by pointer has the same id as the iteratedModel passed through the ctor chain
• void allocate_by_pointer (const String &method_ptr, Iterator &the_iterator, Model &the_model)
  initialize the_iterator and the_model based on method_ptr
• void allocate_by_name (const String &method_string, const String &model_ptr, Iterator &the_iterator, Model &the_model)
  initialize the_iterator based on method_string
• std::pair<int, int> estimate_by_pointer (const String &method_ptr, Iterator &the_iterator, Model &the_model)
  estimate minimum and maximum processors per iterator needed for init_iterator.parallelism(); instantiates the_iterator and the_model as needed, but on minimal processor ranks (is later augmented by allocate_by_pointer())
• std::pair<int, int> estimate_by_name (const String &method_string, const String &model_ptr, Iterator &the_iterator, Model &the_model)
  estimate minimum and maximum processors per iterator needed for init_iterator.parallelism(); instantiates the_iterator and the_model as needed, but on minimal processor ranks (is later augmented by allocate_by_name())

Protected Attributes
• IteratorScheduler iterSched
  scheduler for concurrent execution of Iterators
• int maxIteratorConcurrency
  maximum number of concurrent sub-iterator executions

Additional Inherited Members

13.76.1 Detailed Description
Base class for meta-iterators.
This base class shares code for concurrent and hybrid meta-iterators, where the former supports multi-start and Pareto set iteration and the latter supports sequential, embedded, and collaborative hybrids.

13.76.2 Member Function Documentation
void post_run (std::ostream &s) [protected], [virtual]
post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way.
Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s post_run(), typically after performing its own implementation steps.
Reimplemented from Iterator.
References MetaIterator::iterSched, IteratorScheduler::lead_rank(), and Iterator::print_results().
The documentation for this class was generated from the following files:
13.77 Minimizer Class Reference

Base class for the optimizer and least squares branches of the iterator hierarchy.

Inheritance diagram for Minimizer:

![Inheritance diagram for Minimizer](image)

**Public Member Functions**

- void `constraint_tolerance` (Real constr_tol)
  
  *set the method constraint tolerance (constraintTol)*

- Real `constraint_tolerance` () const
  
  *return the method constraint tolerance (constraintTol)*

- bool `resize` ()
  
  *reinitializes iterator based on new variable size*

**Static Public Member Functions**

- static Real `sum_squared_residuals` (size_t num_pri_fns, const RealVector &residuals, const RealVector &weights)
  
  *return weighted sum of squared residuals*

- static void `print_residuals` (size_t num_terms, const RealVector &best_terms, const RealVector &weights, size_t num_best, size_t best_index, std::ostream &s)
  
  *print num_terms residuals and misfit for final results*
• static void print_model_resp (size_t num_pri_fns, const RealVector &best_fns, size_t num_best, size_t best_index, std::ostream &s)
  print the original user model resp in the case of data transformations

Protected Member Functions
• Minimizer ()
  default constructor
• Minimizer (ProblemDescDB &problem_db, Model &model)
  standard constructor
• Minimizer (unsigned short method_name, Model &model)
  alternate constructor for "on the fly" instantiations
• Minimizer (unsigned short method_name, size_t num_lin_ineq, size_t num_lin_eq, size_t num_nln_ineq, size_t num_nln_eq)
  alternate constructor for "on the fly" instantiations
• ~Minimizer ()
  destructor
• void update_from_model (const Model &model)
  set inherited data attributes based on extractions from incoming model
• void initialize_run ()
  utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
• void post_run (std::ostream &s)
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
• void finalize_run ()
  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
• const Model & algorithm_space_model () const
• Model original_model (unsigned short recasts_left=0)
  Return a shallow copy of the original model this Iterator was originally passed, optionally leaving recasts_left on top of it.
• void data_transform_model ()
  Wrap iteratedModel in a RecastModel that subtracts provided observed data from the primary response functions (variables and secondary responses are unchanged)
• void scale_model ()
  Wrap iteratedModel in a RecastModel that performs variable and/or response scaling.
• Real objective (const RealVector &fn_vals, const BoolDeque &max_sense, const RealVector &primary_wts) const
  compute a composite objective value from one or more primary functions
• Real objective (const RealVector &fn_vals, size_t num_fns, const BoolDeque &max_sense, const RealVector &primary_wts) const
  compute a composite objective with specified number of source primary functions, instead of userPrimaryFns
• void objective_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &max_sense, const RealVector &primary_wts, RealVector &obj_grad) const
  compute the gradient of the composite objective function
• void **objective_gradient** (const RealVector &fn vals, size_t num_fn, const RealMatrix &fn grads, const BoolDeque &max_sense, const RealVector &primary_wts, RealVector &obj_grad) const
  
  compute the gradient of the composite objective function

• void **objective_hessian** (const RealVector &fn vals, const RealMatrix &fn grads, const RealSymMatrixArray &fn_hessians, const BoolDeque &max_sense, const RealVector &primary_wts, RealSymMatrix &obj_hess) const
  
  compute the Hessian of the composite objective function

• void **objective_hessian** (const RealVector &fn vals, size_t num_fn, const RealMatrix &fn grads, const RealSymMatrixArray &fn_hessians, const BoolDeque &max_sense, const RealVector &primary_wts, RealSymMatrix &obj_hess) const
  
  compute the Hessian of the composite objective function

• void **archive_allocate_best** (size_t num_points)
  
  allocate results arrays and labels for multipoint storage

• void **archive_best** (size_t index, const Variables &best_vars, const Response &best_resp)
  
  archive the best point into the results array

• void **resize_best_vars_array** (size_t newsize)
  
  Safely resize the best variables array to newsize taking into account the envelope-letter design pattern and any recasting.

• void **resize_bestResp_array** (size_t newsize)
  
  Safely resize the best response array to newsize taking into account the envelope-letter design pattern and any recasting.

• void **local_recast_retrieve** (const Variables &vars, Response &response) const
  
  infers MOO/NLS solution from the solution of a single-objective optimizer

**Protected Attributes**

- size_t numFunctions
  
  number of response functions

- size_t numContinuousVars
  
  number of active continuous vars

- size_t numDiscreteIntVars
  
  number of active discrete integer vars

- size_t numDiscreteStringVars
  
  number of active discrete string vars

- size_t numDiscreteRealVars
  
  number of active discrete real vars

- Real constraintTol
  
  optimizer/least squares constraint tolerance

- Real bigRealBoundSize
  
  cutoff value for inequality constraint and continuous variable bounds

- int bigIntBoundSize
  
  cutoff value for discrete variable bounds

- size_t numNonlinearIneqConstraints
  
  number of nonlinear inequality constraints
• size_t numNonlinearEqConstraints
  number of nonlinear equality constraints
• size_t numLinearIneqConstraints
  number of linear inequality constraints
• size_t numLinearEqConstraints
  number of linear equality constraints
• size_t numNonlinearConstraints
  total number of nonlinear constraints
• size_t numLinearConstraints
  total number of linear constraints
• size_t numConstraints
  total number of linear and nonlinear constraints
• bool optimizationFlag
  flag for use where optimization and NLS must be distinguished
• size_t numUserPrimaryFns
  number of objective functions or least squares terms in the inbound model; always initialize at Minimizer, even if overridden later
• size_t numIterPrimaryFns
  number of objective functions or least squares terms in iterator’s view, after transformations; always initialize at Minimizer, even if overridden later
• bool boundConstraintFlag
  convenience flag for denoting the presence of user-specified bound constraints. Used for method selection and error checking.
• bool speculativeFlag
  flag for speculative gradient evaluations
• bool calibrationDataFlag
  flag indicating whether user-supplied calibration data is active
• ExperimentData expData
  Container for experimental data to which to calibrate model using least squares or other formulations which minimize SSE.
• size_t numExperiments
  number of experiments
• size_t numTotalCalibTerms
  number of total calibration terms (sum over experiments of number of experimental data per experiment, including field data)
• Model dataTransformModel
  Shallow copy of the data transformation model, when present (cached in case further wrapped by other transformations)
• bool scaleFlag
  whether Iterator-level scaling is active
• Model scalingModel
  Shallow copy of the scaling transformation model, when present (cached in case further wrapped by other transformations)
• Minimizer * prevMinInstance
Static Protected Attributes

- static Minimizer * minimizerInstance
  pointer to Minimizer used in static member functions

Friends

- class SOLBase
  the SOLBase class is not derived the iterator hierarchy but still needs access to iterator hierarchy data (to avoid attribute replication)

- class SNLLBase
  the SNLLBase class is not derived the iterator hierarchy but still needs access to iterator hierarchy data (to avoid attribute replication)

Additional Inherited Members

13.77.1 Detailed Description

Base class for the optimizer and least squares branches of the iterator hierarchy.

The Minimizer class provides common data and functionality for Optimizer and LeastSq.

13.77.2 Constructor & Destructor Documentation

Minimizer (ProblemDescDB & problem_db, Model & model) [protected]

standard constructor

This constructor extracts inherited data for the optimizer and least squares branches and performs sanity checking on constraint settings.

References Iterator::iteratedModel, Iterator::maxIterations, Iterator::methodName, Iterator::numFinalSolutions, and Minimizer::update

from model().

13.77.3 Member Function Documentation

void initialize_run() [protected], [virtual]

utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s initialize_run(), typically before performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in SNLLOptimizer, NLPQLPOptimizer, SNLLLeastSq, DOTOptimizer, and Optimizer.

References Model::all_continuous_variables(), Model::all_discrete_int_variables(), Model::all_discrete_real_variables(), Iterator::bestVariablesArray, Model::initialize_mapping(), Model::is_null(), Iterator::iteratedModel, Model::mapping_initialized(), Iterator::methodPCIter, Minimizer::minimizerInstance, Iterator::myModelLayers,
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Minimizer::prevMinInstance, Minimizer::resize(), Model::set_evaluation_reference(), Iterator::subIteratorFlag, Model::subordinate_model(), and Iterator::summaryOutputFlag.

Referenced by LeastSq::initialize_run(), and Optimizer::initialize_run().

```cpp
void post_run ( std::ostream & s ) [protected], [virtual]
```

Post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way.

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s `post_run()`, typically after performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in SNLLOptimizer, SNLLLeastSq, Optimizer, SurrBasedLocalMinimizer, DataFitSurrBasedLocalMinimizer, and HierarchSurrBasedLocalMinimizer.

References Model::is_null(), Iterator::iteratedModel, Model::print_evaluation_summary(), Iterator::print_results(), Iterator::resultsDB, Iterator::summaryOutputFlag, and ResultsManager::write_databases().

Referenced by LeastSq::post_run(), SurrBasedLocalMinimizer::post_run(), Optimizer::post_run(), and SNLLLeastSq::post_run().

```cpp
void finalize_run ( ) [protected], [virtual]
```

Utility function to perform common operations following `post_run()`: deallocation and resetting of instance pointers.

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s `finalize_run()`, typically after performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in SNLLOptimizer, SNLLLeastSq, and Optimizer.

References Model::finalize_mapping(), Iterator::finalize_run(), Iterator::iteratedModel, Model::mapping_initialized(), Minimizer::minimizerInstance, Minimizer::prevMinInstance, and Minimizer::resize().

Referenced by LeastSq::finalize_run(), and Optimizer::finalize_run().

```cpp
const Model & algorithm_space_model ( ) const [inline], [protected], [virtual]
```

Default definition that gets redefined in selected derived Minimizers.

Reimplemented from Iterator.

Reimplemented in EffGlobalMinimizer.

References Iterator::iteratedModel.

```cpp
void data_transform_model ( ) [protected]
```

Wrap `iteratedModel` in a `RecastModel` that subtracts provided observed data from the primary response functions (variables and secondary responses are unchanged).

Reads observation data to compute least squares residuals. Does not change size of responses, and is the first wrapper, therefore sizes are based on `iteratedModel`.

References Dakota::abort_handler(), Iterator::activeSet, Iterator::assign_rep(), Minimizer::dataTransformModel, Minimizer::expData, ProblemDescDB::get_sizet(), Iterator::iteratedModel, ExperimentData::load_data(), Iterator::myModelLayers, Model::num_functions(), Model::num_primary_fns(), Minimizer::numExperiments, Minimizer::numFunctions, Minimizer::numIterPrimaryFns, Minimizer::numTotalCalibTerms, Iterator::outputLevel, Iterator::probDescDB, and ActiveSet::request_vector().

Referenced by LeastSq::LeastSq(), and Optimizer::Optimizer().
void scale_model ( ) [protected]

Wrap iteratedModel in a RecastModel that performs variable and/or response scaling.
- Wrap the iteratedModel in a scaling transformation, such that iteratedModel now contains a scaling recast model. Potentially affects variables, primary, and secondary responses.
- References Model::assign_rep(), Iterator::iteratedModel, Iterator::myModelLayers, and Minimizer::scalingModel.
- Referenced by LeastSq::LeastSq(), and Optimizer::Optimizer().

Real objective ( const RealVector & fn_vals, const BoolDeque & max_sense, const RealVector & primary_wts ) const [protected]

compute a composite objective value from one or more primary functions
- The composite objective computation sums up the contributions from one of more primary functions using the primary response fn weights.
- References Minimizer::numUserPrimaryFns.
- Referenced by SurrBasedLocalMinimizer::approx_subprob_objective_eval(), SurrBasedMinimizer::augmented_lagrangian_merit(), EffGlobalMinimizer::expected_improvement(), SurrBasedMinimizer::initialize_filter(), Surr-BasedMinimizer::lagrangian_merit(), Optimizer::objective_reduction(), SurrBasedMinimizer::penalty_merit(), COLINOptimizer::post_run(), SurrBasedMinimizer::update_filter(), and SurrBasedLocalMinimizer::update_penalty().

Real objective ( const RealVector & fn_vals, size_t num_fns, const BoolDeque & max_sense, const RealVector & primary_wts ) const [protected]

compute a composite objective with specified number of source primary functions, instead of userPrimaryFns
- This "composite" objective is a more general case of the previous objective(), but doesn’t presume a reduction map from user to iterated space. Used to apply weights and sense in COLIN results sorting. Leaving as a duplicate implementation pending resolution of COLIN lookups.
- References Minimizer::optimizationFlag.

void objective_gradient ( const RealVector & fn_vals, size_t num_fns, const RealMatrix & fn_grads, const BoolDeque & max_sense, const RealVector & primary_wts, RealVector & obj_grad ) const [protected]

compute the gradient of the composite objective function
- The composite objective gradient computation combines the contributions from one of more primary function gradients, including the effect of any primary function weights. In the case of a linear mapping (MOO), only the primary function gradients are required, but in the case of a nonlinear mapping (NLS), primary function values are also needed. Within RecastModel::set_mapping(), the active set requests are automatically augmented to make values available when needed, based on nonlinearRespMapping settings.
- References Minimizer::numContinuousVars, and Minimizer::optimizationFlag.

void objective_hessian ( const RealVector & fn_vals, size_t num_fns, const RealMatrix & fn_grads, const RealSymMatrixArray & fn_hessians, const BoolDeque & max_sense, const RealVector & primary_wts, RealSymMatrix & obj_hess ) const [protected]

compute the Hessian of the composite objective function
- The composite objective Hessian computation combines the contributions from one of more primary function Hessians, including the effect of any primary function weights. In the case of a linear mapping (MOO), only the primary function Hessians are required, but in the case of a nonlinear mapping (NLS), primary function values and gradients are also needed in general (gradients only in the case of a Gauss-Newton approximation). Within
the default RecastModel::set_mapping(), the active set requests are automatically augmented to make values and
gradients available when needed, based on nonlinearRespMapping settings.

References Dakota::abort_handler(), Minimizer::numContinuousVars, and Minimizer::optimizationFlag.

```cpp
void resize_best_vars_array ( size_t newsize ) [protected]
```

Safely resize the best variables array to newsize taking into account the envelope-letter design pattern and any
recasting.

Uses data from the innermost model, should any Minimizer recasts be active. Called by multipoint return
solvers. Do not directly call resize on the bestVariablesArray object unless you intend to share the internal content
(letter) with other objects after assignment.

References Iterator::bestVariablesArray, Variables::copy(), Model::current_variables(), and Minimizer::original-
_model().

Referenced by COLINOptimizer::post_run().

```cpp
void resize_best_resp_array ( size_t newsize ) [protected]
```

Safely resize the best response array to newsize taking into account the envelope-letter design pattern and any
recasting.

Uses data from the innermost model, should any Minimizer recasts be active. Called by multipoint return
solvers. Do not directly call resize on the bestResponseArray object unless you intend to share the internal content
(letter) with other objects after assignment.

References Iterator::bestResponseArray, Response::copy(), Model::current_response(), and Minimizer::original-
_model().

Referenced by COLINOptimizer::post_run().

```cpp
void local_recast_retrieve ( const Variables & vars, Response & response ) const [protected]
```

infers MOO/NLS solution from the solution of a single-objective optimizer

Retrieve a MOO/NLS response based on the data returned by a single objective optimizer by performing a
data_pairs search. This may get called even for a single user-specified function, since we may be recasting a single
NLS residual into a squared objective. Always returns best data in the space of the original inbound Model.

References Response::active_set(), Dakota::data_pairs, Model::interface_id(), Iterator::iteratedModel, Dakota-
::lookup_by_val(), and Response::update().

Referenced by LeastSq::post_run(), and Optimizer::post_run().

The documentation for this class was generated from the following files:

- DakotaMinimizer.hpp
- DakotaMinimizer.cpp

### 13.78 MixedVarConstraints Class Reference

Derived class within the Constraints hierarchy which separates continuous and discrete variables (no domain type
array merging).

Inheritance diagram for MixedVarConstraints:
**Public Member Functions**

- **MixedVarConstraints** (const `SharedVariablesData` &svd)
  
  *lightweight constructor*

- **MixedVarConstraints** (const `ProblemDescDB` &problem_db, const `SharedVariablesData` &svd)
  
  *standard constructor*

- `~MixedVarConstraints` ()
  
  *destructor*

- void `write` (std::ostream &s) const
  
  *write a variable constraints object to an std::ostream*

- void `read` (std::istream &s)
  
  *read a variable constraints object from an std::istream*

**Additional Inherited Members**

**13.78.1 Detailed Description**

Derived class within the `Constraints` hierarchy which separates continuous and discrete variables (no domain type array merging).

Derived variable constraints classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The `MixedVarConstraints` derived class separates the continuous and discrete domain types (see `Variables::get_variables(problem_db)` for variables type selection; variables type is passed to the `Constraints` constructor in `Model`).

**13.78.2 Constructor & Destructor Documentation**

`MixedVarConstraints` ( const `ProblemDescDB` & `problem_db`, const `SharedVariablesData` & `svd` )

*standard constructor*

In this class, mixed continuous/discrete variables are used. Most iterators/strategies use this approach, which is the default in `Constraints::get_constraints()`.

References `Constraints::allContinuousLowerBnds`, `Constraints::allContinuousUpperBnds`, `Constraints::allDiscreteIntLowerBnds`, `Constraints::allDiscreteIntUpperBnds`, `Constraints::allDiscreteRealLowerBnds`, `Constraints::allDiscreteRealUpperBnds`, `Dakota::copy_data::partial()`, `ProblemDescDB::get_iv()`, `ProblemDescDB::get_rv()`, `Constraints::sharedVarsData`, and `SharedVariablesData::view()`.

The documentation for this class was generated from the following files:

- `MixedVarConstraints.hpp`
- `MixedVarConstraints.cpp`
13.79 MixedVariables Class Reference

Derived class within the Variables hierarchy which separates continuous and discrete variables (no domain type array merging).

Inheritance diagram for MixedVariables:

```
Variables
  ▼
 MixedVariables
```

Public Member Functions

- MixedVariables (const ProblemDescDB &problem_db, const std::pair< short, short >&view)  
  standard constructor
- MixedVariables (const SharedVariablesData &svd)  
  lightweight constructor
- ~MixedVariables ()  
  destructor

Protected Member Functions

- void read (std::istream &s)  
  read a variables object from an std::istream
- void write (std::ostream &s, unsigned short vars_part=ALL_VARS) const  
  write a variables object to an std::ostream, e.g., the console, optionally specifying which partition (all/active/inactive)
- void write_aprepro (std::ostream &s) const  
  write a variables object to an std::ostream in aprepro format, e.g., a parameters file
- void read_tabular (std::istream &s, unsigned short vars_part=ALL_VARS)  
- void write_tabular (std::ostream &s, unsigned short vars_part=ALL_VARS) const  
- void write_tabular_labels (std::ostream &s, unsigned short vars_part=ALL_VARS) const  
- template<typename Reader > void read_core (std::istream &s, Reader read_handler, unsigned short vars_part)  
  Implementation of reading various formats using the specified read handler.
- template<typename Writer > void write_core (std::ostream &s, Writer write_handler, unsigned short vars_part) const  
  Implementation of writing various formats using the specified write handler.
Additional Inherited Members

13.79.1 Detailed Description

Derived class within the Variables hierarchy which separates continuous and discrete variables (no domain type array merging).

Derived variables classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The MixedVariables derived class separates the continuous and discrete domain types (see Variables::get_variables(problem_db)).

13.79.2 Constructor & Destructor Documentation

MixedVariables ( const ProblemDescDB & problem_db, const std::pair< short, short > & view )

standard constructor

In this class, the distinct approach is used (design, uncertain, and state variable types and continuous and discrete domain types are distinct). Most iterators/strategies use this approach.

References Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, Dakota::copy_data_partial(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), ProblemDescDB::get_sa(), Variables::sharedVarsData, and SharedVariablesData::view().

13.79.3 Member Function Documentation

void read_tabular ( std::istream & s, unsigned short vars_part = ALL_VARS ) [protected], [virtual]

Tabular reader that reads data in order design, aleatory, epistemic, state according to counts in vc_totals (extract in order: cdv/ddv/drdrv, cauv/dauv/dauv, ceuv/deuiv/deurv, csv/dsv/dsrv, which might reflect active or all depending on context. Assumes container sized, since might be a view into a larger array.

Reimplemented from Variables.

References MixedVariables::read_core().

void read_core ( std::istream & s, Reader read_handler, unsigned short vars_part ) [protected]

Implementation of reading various formats using the specified read handler.

Reordering is required in all read/write cases that will be visible to the user since all derived vars classes should use the same CDV/DDV/UV/CSV/DSV ordering for clarity. Neutral file I/O, binary streams, and packed buffers do not need to reorder (so long as read/write are consistent) since this data is not intended for public consumption.

References SharedVariablesData::active_components_totals(), Variables::all_continuous_variable_labels(), Variables::all_discrete_int_variable_labels(), Variables::all_discrete_real_variable_labels(), Variables::all_discrete_string_variable_labels(), Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, SharedVariablesData::components_totals(), SharedVariablesData::cv_start(), SharedVariablesData::div_start(), SharedVariablesData::drv_start(), SharedVariablesData::dsv_start(), SharedVariablesData::icv_start(), SharedVariablesData::idrv_start(), SharedVariablesData::idsv_start(), SharedVariablesData::inactive_components_totals(), and Variables::sharedVarsData.

Referenced by MixedVariables::read(), and MixedVariables::read_tabular().

The documentation for this class was generated from the following files:

- MixedVariables.hpp
- MixedVariables.cpp
13.80 Model Class Reference

Base class for the model class hierarchy.

Inheritance diagram for Model:

```
Model
  NestedModel  
  RecastModel
  SimulationModel
  SurrogateModel
    ActiveSubspaceModel
    AdaptedBasisModel
    DataTransformModel
    ProbabilityTransformModel
    RandomFieldModel
    ScalingModel
    DataFitSurrModel
    HierarchSurrModel
```

Public Member Functions

- **Model ()**
  
  default constructor

- **Model (ProblemDescDB &problem_db)**

  standard constructor for envelope

- **Model (const Model &model)**

  copy constructor

- **virtual ~Model ()**

  destructor

- **Model operator= (const Model &model)**

  assignment operator

- **virtual Iterator & subordinate_iterator ()**

  return the sub-iterator in nested and surrogate models

- **virtual Model & subordinate_model ()**

  return a single sub-model defined from subModel in nested and recast models and truth_model() in surrogate models; used for a directed dive through model recursions that may bypass some components.

- **virtual Model & surrogate_model ()**

  return the active approximation sub-model in surrogate models

- **virtual void surrogate_model_indices (size_t lf_model_index, size_t lf_soln_lev_index=_NPOS)**

  set the indices that define the active approximation sub-model within surrogate models

- **virtual void surrogate_model_indices (const SizetSizetPair &lf_form_level)**

  set the index pair that defines the active approximation sub-model within surrogate models

- **virtual const SizetSizetPair & surrogate_model_indices () const**

  return the indices of the active approximation sub-model within surrogate models

- **virtual Model & truth_model ()**

  return the active truth sub-model in surrogate models
• virtual void truth_model_indices (size_t hf_model_index, size_t hf_soln_lev_index=NPOS)
  set the indices that define the active truth sub-model within surrogate models
• virtual void truth_model_indices (const SizetSizetPair &hf_form_level)
  set the index pair that defines the active truth sub-model within surrogate models
• virtual const SizetSizetPair & truth_model_indices () const
  return the indices of the active truth sub-model within surrogate models
• virtual void derived_subordinate_models (ModelList &ml, bool recurse_flag)
  portion of subordinate_models() specific to derived model classes
• virtual void update_from_subordinate_model (size_t depth=std::numeric_limits<size_t>::max())
  propagate vars/labels/bounds/targets from the bottom up
• virtual Interface & derived_interface ()
  return the interface employed by the derived model class, if present: SimulationModel::userDefinedInterface, Data-FitSurrModel::approxInterface, or NestedModel::optionalInterface
• virtual size_t solution_levels () const
  number of discrete levels within solution control (SimulationModel)
• virtual void solution_level_index (size_t index)
  activate a particular level within the solution level control and return the cost estimate (SimulationModel)
• virtual RealVector solution_level_cost () const
  return ordered cost estimates across solution levels (SimulationModel)
• virtual void primary_response_fn_weights (const RealVector &wts, bool recurse_flag=true)
  set the relative weightings for multiple objective functions or least squares terms
• virtual void surrogate_function_indices (const IntSet &surr_fn_indices)
  set the (currently active) surrogate function index set
• virtual bool initialize_mapping (ParLevLIter pl_iter)
  initialize model mapping, returns true if the variables size has changed
• virtual bool finalize_mapping ()
  finalize model mapping, returns true if the variables size has changed
• virtual bool mapping_initialized () const
  return true if mapping has been fully initialized, false otherwise.
• virtual bool resize_pending () const
  return true if a potential resize is still pending, such that sizing-based initialization should be deferred
• virtual void build_approximation ()
  build a new SurrogateModel approximation
• virtual bool build_approximation (const Variables &vars, const IntResponsePair &response_pr)
  build a new SurrogateModel approximation using/enforcing anchor response at vars; rebuild if needed
• virtual void update_approximation (bool rebuild_flag)
  replace the approximation data within an existing surrogate based on data updates propagated elsewhere
• virtual void update_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)
  replace the anchor point data within an existing surrogate
• virtual void update_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)
  replace the data points within an existing surrogate
virtual void update_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_flag)
    replace the data points within an existing surrogate

virtual void append_approximation (bool rebuild_flag)
    append to the existing approximation data within a surrogate based on data updates propagated elsewhere

virtual void append_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)
    append a single point to an existing surrogate’s data

virtual void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)
    append multiple points to an existing surrogate’s data

virtual void append_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_flag)
    append multiple points to an existing surrogate’s data

virtual void pop_approximation (bool save_surr_data, bool rebuild_flag=false)
    remove the previous data set addition to a surrogate (e.g., due to a previous append_approximation() call); flag manages storing of surrogate data for use in a subsequent push_approximation()

virtual void push_approximation ()
    push a previous approximation data state; reverse of pop_approximation

virtual bool push_available ()
    query for whether a trial increment is restorable within a surrogate

virtual void finalize_approximation ()
    finalize an approximation by applying all previous trial increments

virtual void store_approximation (size_t index=NPOS)
    move the current approximation into storage for later combination; the index of the stored set can be passed to allow replacement instead of augmentation (default is push_back)

virtual void restore_approximation (size_t index=NPOS)
    return an approximation from storage; the index identifies a particular stored data set (default is pop_back from stored)

virtual void remove_stored_approximation (size_t index=NPOS)
    remove a stored approximation, due to redundancy with the current approximation, prior to combination (default for no index is pop_back)

virtual void combine_approximation (short corr_type)
    combine the current approximation with previously stored data sets

virtual void run_dace_iterator (bool rebuild_flag)
    execute the DACE iterator; append the approximation data, and rebuild the approximation if indicated

virtual bool force_rebuild ()
    determine whether a surrogate model rebuild should be forced based on changes in the inactive data

virtual SharedApproxData & shared_approximation ()
    retrieve the shared approximation data within the ApproximationInterface of a DataFitSurrModel

virtual std::vector<Approximation> & approximations ()
    retrieve the set of Approximations within the ApproximationInterface of a DataFitSurrModel

virtual const Pecos::SurrogateData & approximation_data (size_t index)
retrieved in DataFitSurfModel.

• virtual const RealVectorArray & approximation_coefficients (bool normalized=false)
  retrieve the approximation coefficients from each Approximation within a DataFitSurfModel

• virtual void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)
  set the approximation coefficients for each Approximation within a DataFitSurfModel

• virtual const RealVector & approximation_variances (const Variables &vars)
  retrieve the prediction variances from each Approximation within a DataFitSurfModel

• virtual void surrogate_response_mode (short mode)
  set response computation mode used in SurrogateModels for forming currentResponse

• virtual short surrogate_response_mode () const
  return response computation mode used in SurrogateModels for forming currentResponse

• virtual const RealVector & error_estimates ()
  retrieve error estimates corresponding to the Model’s response (could be surrogate error for SurrogateModels,
statistical MSE for NestedModels, or adjoint error estimates for SimulationModels). Errors returned correspond to
most recent evaluate().

• virtual DiscrepancyCorrection & discrepancy_correction ()
  return the DiscrepancyCorrection object used by SurrogateModels

• virtual void single_apply (const Variables &vars, Response &resp, const SizetSizet2DPair &indices)
  apply the DiscrepancyCorrection object to correct an approximation within a SurrogateModel

• virtual void recursive_apply (const Variables &vars, Response &resp)
  apply the DiscrepancyCorrection object to recursively correct an approximation within a HierarchSurrModel

• virtual void component_parallel_mode (short mode)
  update componentParallelMode for supporting parallelism in model sub-components

• virtual IntIntPair estimate_partition_bounds (int max_eval_concurrency)
  estimate the minimum and maximum partition sizes that can be utilized by this Model

• virtual size_t mi_parallel_level_index () const
  return the index for the metaiterator-iterator parallelism level within ParallelConfiguration::miPLIters that is active
for use in a particular Model at runtime

• virtual void cache_unmatched_response (int raw_id)
  migrate an unmatched response record from active response map (computed by synchronize() or synhronize_-nowait()) to cached response map

• virtual short local_eval_synchronization ()
  return derived model synchronization setting

• virtual int local_eval_concurrency ()
  return derived model asynchronous evaluation concurrency

• virtual void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)
  Service job requests received from the master. Completes when a termination message is received from stop._servers().

• virtual void stop_servers ()
  Executed by the master to terminate all server operations for a particular model when iteration on the model is
complete.

• virtual bool derived_master_overload () const
  Return a flag indicating the combination of multiprocessor evaluations and a dedicated master iterator scheduling.
Used in synchronous evaluate functions to prevent the error of trying to run a multiprocessor job on the master.
• virtual void inactive_view (short view, bool recurse_flag=true)
  update the Model’s inactive view based on higher level (nested) context
• virtual const String & interface_id () const
  return the interface identifier
• virtual int derived_evaluation_id () const
  Return the value of the evaluation id counter for the Model.
• virtual bool evaluation_cache (bool recurse_flag=true) const
  Indicates the usage of an evaluation cache by the Model.
• virtual bool restart_file (bool recurse_flag=true) const
  Indicates the usage of a restart file by the Model.
• virtual void set_evaluation_reference ()
  Set the reference points for the evaluation counters within the Model.
• virtual void fine_grained_evaluation_counters ()
  Request fine-grained evaluation reporting within the Model.
• virtual void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const
  Print an evaluation summary for the Model.
• virtual void eval_tag_prefix (const String &eval_id_str)
  set the hierarchical eval ID tag prefix
• virtual bool db_lookup (const Variables &search_vars, const ActiveSet &search_set, Response &found_resp)
  search the eval database (during derivative estimation); derived may need to reimplement due to problem transformations (RecastModel); return true if found in DB
• virtual void stop_init_mapping (ParLevLIter pl_iter)
  called from IteratorScheduler::run_iterator() for iteratorComm rank 0 to terminate serve_init_mapping() on other iteratorComm processors
• virtual int serve_init_mapping (ParLevLIter pl_iter)
  called from IteratorScheduler::run_iterator() for iteratorComm rank != 0 to balance resize() calls on iteratorComm rank 0
• virtual void stop_finalize_mapping (ParLevLIter pl_iter)
  called from IteratorScheduler::run_iterator() for iteratorComm rank 0 to terminate serve_finalize_mapping() on other iteratorComm processors
• virtual int serve_finalize_mapping (ParLevLIter pl_iter)
  called from IteratorScheduler::run_iterator() for iteratorComm rank != 0 to balance resize() calls on iteratorComm rank 0
• virtual void warm_start_flag (const bool flag)
  set the warm start flag (warmStartFlag)
• ModelList & subordinate_models (bool recurse_flag=true)
  return the sub-models in nested and surrogate models
• void evaluate ()
  Compute the Response at currentVariables (default ActiveSet).
• void evaluate (const ActiveSet &set)
  Compute the Response at currentVariables (specified ActiveSet).
• void evaluate_nowait ()
Spawn an asynchronous job (or jobs) that computes the value of the `Response` at `currentVariables` (default `ActiveSet`).

- `void evaluate_nowait (const ActiveSet &set)`
  Spawn an asynchronous job (or jobs) that computes the value of the `Response` at `currentVariables` (specified `ActiveSet`).

- `const IntResponseMap & synchronize ()`
  Execute a blocking scheduling algorithm to collect the complete set of results from a group of asynchronous evaluations.

- `const IntResponseMap & synchronize_nowait ()`
  Execute a nonblocking scheduling algorithm to collect all available results from a group of asynchronous evaluations.

- `int evaluation_id () const`
  return Model’s (top-level) evaluation counter, not to be confused with derived counter returned by `derived_evaluation_id()`

- `void init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)`
  allocate communicator partitions for a model and store configuration in modelPCIterMap

- `void init_serial ()`
  for cases where `init_communicators()` will not be called, modify some default settings to behave properly in serial.

- `void set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)`
  set active parallel configuration for the model (set modelPCIter from modelPCIterMap)

- `void free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)`
  deallocate communicator partitions for a model

- `MPI_Comm analysis_comm () const`
  retrieve the MPI communicator on which this model is configured to conduct function evaluation analyses (provided for library clients)

- `void stop_init_communicators (ParLevLIter pl_iter)`
  called from `IteratorScheduler::init_iterator()` for iteratorComm rank 0 to terminate `serve_init_communicators()` on other iteratorComm processors

- `int serve_init_communicators (ParLevLIter pl_iter)`
  called from `IteratorScheduler::init_iterator()` for iteratorComm rank != 0 to balance `init_communicators()` calls on iteratorComm rank 0

- `void estimate_message_lengths ()`
  estimate messageLengths for a model

- `bool manage_data_recastings ()`
  initialize modelList and recastFlags for data import/export

- `bool recastings () const`
  return true if recastFlags is defined

- `void user_space_to_iterator_space (const Variables &user_vars, const Response &user_resp, Variables &iter_vars, Response &iter_resp)`
  employ the model recursion to transform from bottom level user-space data to top level iterator-space data

- `void iterator_space_to_user_space (const Variables &iter_vars, const Response &iter_resp, Variables &user_vars, Response &user_resp)`
  employ the model recursion to transform from top level iterator-space data to bottom level user-space data

- `void assign_rep (Model *model_rep, bool ref_count_incr=true)`
  replaces existing letter with a new one
CHAPTER 13. CLASS DOCUMENTATION

- `size_t tv () const`
  returns total number of vars

- `size_t cv () const`
  returns number of active continuous variables

- `size_t div () const`
  returns number of active discrete integer vars

- `size_t dsv () const`
  returns number of active discrete string vars

- `size_t drv () const`
  returns number of active discrete real vars

- `size_t icv () const`
  returns number of inactive continuous variables

- `size_t idiv () const`
  returns number of inactive discrete integer vars

- `size_t idsv () const`
  returns number of inactive discrete string vars

- `size_t idrv () const`
  returns number of inactive discrete real vars

- `size_t acv () const`
  returns total number of continuous variables

- `size_t adiv () const`
  returns total number of discrete integer vars

- `size_t adsv () const`
  returns total number of discrete string vars

- `size_t adrv () const`
  returns total number of discrete real vars

- `void active_variables (const Variables &vars)`
  set the active variables in currentVariables

- `const RealVector & continuous_variables () const`
  return the active continuous variables from currentVariables

- `const Real continuous_variable (size_t i) const`
  return an active continuous variable from currentVariables

- `void continuous_variables (const RealVector &c_vars)`
  set the active continuous variables in currentVariables

- `void continuous_variable (Real c_var, size_t i)`
  set an active continuous variable in currentVariables

- `const IntVector & discrete_int_variables () const`
  return the active discrete integer variables from currentVariables

- `int discrete_int_variable (size_t i) const`
  return an active discrete integer variable from currentVariables

- `void discrete_int_variables (const IntVector &d_vars)`
  set the active discrete integer variables in currentVariables

- `void discrete_int_variable (int d_var, size_t i)`
set an active discrete integer variable in currentVariables

- StringMultiArrayConstView discrete_string_variables() const
  return the active discrete string variables from currentVariables

- const String & discrete_string_variable(size_t i) const
  return an active discrete string variable from currentVariables

- void discrete_string_variables(StringMultiArrayConstView d_vars)
  set the active discrete string variables in currentVariables

- void discrete_string_variable(const String &d_var, size_t i)
  set an active discrete string variable in currentVariables

- const RealVector & discrete_real_variables() const
  return the active discrete real variables from currentVariables

- Real discrete_real_variable(size_t i) const
  return an active discrete real variable from currentVariables

- void discrete_real_variables(const RealVector &d_vars)
  set the active discrete real variables in currentVariables

- void discrete_real_variable(Real d_var, size_t i)
  set an active discrete real variable in currentVariables

- UShortMultiArrayConstView continuous_variable_types() const
  return the active continuous variable types from currentVariables

- void continuous_variable_types(UShortMultiArrayConstView cv_types)
  set the active continuous variable types in currentVariables

- void continuous_variable_type(unsigned short cv_type, size_t i)
  set an active continuous variable type in currentVariables

- UShortMultiArrayConstView discrete_int_variable_types() const
  return the active discrete variable types from currentVariables

- void discrete_int_variable_types(UShortMultiArrayConstView div_types)
  set the active discrete variable types in currentVariables

- void discrete_int_variable_type(unsigned short div_type, size_t i)
  set an active discrete variable type in currentVariables

- UShortMultiArrayConstView discrete_string_variable_types() const
  return the active discrete variable types from currentVariables

- void discrete_string_variable_types(UShortMultiArrayConstView drv_types)
  set the active discrete variable types in currentVariables

- void discrete_string_variable_type(unsigned short drv_type, size_t i)
  set an active discrete variable type in currentVariables

- UShortMultiArrayConstView discrete_real_variable_types() const
  return the active discrete variable types from currentVariables

- void discrete_real_variable_types(UShortMultiArrayConstView drv_types)
  set the active discrete variable types in currentVariables

- void discrete_real_variable_type(unsigned short drv_type, size_t i)
  set an active discrete variable type in currentVariables

- SizetMultiArrayConstView continuous_variable_ids() const
  return the active continuous variable identifiers from currentVariables
• void continuous_variable_ids (SizetMultiArrayConstView cv_ids)
  set the active continuous variable identifiers in currentVariables
• void continuous_variable_id (size_t cv_id, size_t i)
  set an active continuous variable identifier in currentVariables
• const RealVector & inactive_continuous_variables () const
  return the inactive continuous variables in currentVariables
• void inactive_continuous_variables (const RealVector &i_c_vars)
  set the inactive continuous variables in currentVariables
• const IntVector & inactive_discrete_int_variables () const
  return the inactive discrete variables in currentVariables
• void inactive_discrete_int_variables (const IntVector &i_d_vars)
  set the inactive discrete variables in currentVariables
• StringMultiArrayConstView inactive_discrete_string_variables () const
  return the inactive discrete string variables in currentVariables
• void inactive_discrete_string_variables (StringMultiArrayConstView i_d_vars)
  set the inactive discrete string variables in currentVariables
• const RealVector & inactive_discrete_real_variables () const
  return the inactive discrete real variables in currentVariables
• void inactive_discrete_real_variables (const RealVector &i_d_vars)
  set the inactive discrete real variables in currentVariables
• UShortMultiArrayConstView inactive_continuous_variable_types () const
  return the inactive continuous variable types from currentVariables
• SizetMultiArrayConstView inactive_continuous_variable_ids () const
  return the inactive continuous variable identifiers from currentVariables
• const RealVector & all_continuous_variables () const
  return all continuous variables in currentVariables
• void all_continuous_variables (const RealVector &a_c_vars)
  set all continuous variables in currentVariables
• void all_continuous_variable (Real a_c_var, size_t i)
  set a variable within the all continuous variables in currentVariables
• const IntVector & all_discrete_int_variables () const
  return all discrete variables in currentVariables
• void all_discrete_int_variables (const IntVector &a_d_vars)
  set all discrete variables in currentVariables
• void all_discrete_int_variable (int a_d_var, size_t i)
  set a variable within the all discrete variables in currentVariables
• StringMultiArrayConstView all_discrete_string_variables () const
  return all discrete string variables in currentVariables
• void all_discrete_string_variables (StringMultiArrayConstView a_d_vars)
  set all discrete variables in currentVariables
• void all_discrete_string_variable (const String &a_d_var, size_t i)
  set a variable within the all discrete variables in currentVariables
• const RealVector & all_discrete_real_variables () const
return all discrete variables in currentVariables

void all_discrete_real_variables (const RealVector &a_d_vars)

set all discrete variables in currentVariables

void all_discrete_real_variable (Real a_d_var, size_t i)

set a variable within the all discrete variables in currentVariables

UShortMultiArrayConstView all_continuous_variable_types () const

return all continuous variable types from currentVariables

UShortMultiArrayConstView all_discrete_int_variable_types () const

return all discrete variable types from currentVariables

UShortMultiArrayConstView all_discrete_string_variable_types () const

return all discrete variable types from currentVariables

UShortMultiArrayConstView all_discrete_real_variable_types () const

return all discrete variable types from currentVariables

UShortMultiArrayConstView all_continuous_variable_ids () const

return all continuous variable identifiers from currentVariables

const IntSetArray & discrete_design_set_int_values () const

return the sets of values available for each of the discrete design set integer variables

void discrete_design_set_int_values (const IntSetArray &isa)

define the sets of values available for each of the discrete design set integer variables

const StringSetArray & discrete_design_set_string_values () const

return the sets of values available for each of the discrete design set string variables

void discrete_design_set_string_values (const StringSetArray &ssa)

define the sets of values available for each of the discrete design set string variables

const RealSetArray & discrete_design_set_real_values () const

return the sets of values available for each of the discrete design set real variables

void discrete_design_set_real_values (const RealSetArray &rsa)

define the sets of values available for each of the discrete design set real variables

const IntSetArray & discrete_state_set_int_values () const

return the sets of values available for each of the discrete state set integer variables

void discrete_state_set_int_values (const IntSetArray &isa)

define the sets of values available for each of the discrete state set integer variables

const StringSetArray & discrete_state_set_string_values () const

return the sets of values available for each of the discrete state set string variables

void discrete_state_set_string_values (const StringSetArray &ssa)

define the sets of values available for each of the discrete state set string variables

const RealSetArray & discrete_state_set_real_values () const

return the sets of values available for each of the discrete state set real variables

void discrete_state_set_real_values (const RealSetArray &rsa)

define the sets of values available for each of the discrete state set real variables

const BitArray & discrete_int_sets ()

define and return discreteIntSets using active view from currentVariables

const BitArray & discrete_int_sets (short active_view)

define and return discreteIntSets using passed active view
• const IntSetArray & discrete_set_int_values ()
  return the sets of values available for each of the active discrete set integer variables (aggregated in activeDiscSetIntValues)
• const IntSetArray & discrete_set_int_values (short active_view)
  return the sets of values available for each of the active discrete set integer variables (aggregated in activeDiscSetIntValues)
• const StringSetArray & discrete_set_string_values ()
  return the sets of values available for each of the active discrete set string variables (aggregated in activeDiscSetStringValues)
• const StringSetArray & discrete_set_string_values (short active_view)
  return the sets of values available for each of the active discrete set string variables (aggregated in activeDiscSetStringValues)
• const RealSetArray & discrete_set_real_values ()
  return the sets of values available for each of the active discrete set real variables (aggregated in activeDiscSetRealValues)
• const RealSetArray & discrete_set_real_values (short active_view)
  return the sets of values available for each of the active discrete set real variables (aggregated in activeDiscSetRealValues)
• Pecos::AleatoryDistParams & aleatory_distribution_parameters ()
  return aleatDistParams
• const Pecos::AleatoryDistParams & aleatory_distribution_parameters () const
  return aleatDistParams
• void aleatory_distribution_parameters (const Pecos::AleatoryDistParams &adp)
  set aleatDistParams
• Pecos::EpistemicDistParams & epistemic_distribution_parameters ()
  return epistDistParams
• const Pecos::EpistemicDistParams & epistemic_distribution_parameters () const
  return epistDistParams
• void epistemic_distribution_parameters (const Pecos::EpistemicDistParams &edp)
  set epistDistParams
• StringMultiArrayConstView continuous_variable_labels () const
  return the active continuous variable labels from currentVariables
• void continuous_variable_labels (StringMultiArrayConstView c_v_labels)
  set the active continuous variable labels in currentVariables
• StringMultiArrayConstView discrete_int_variable_labels () const
  return the active discrete variable labels from currentVariables
• void discrete_int_variable_labels (StringMultiArrayConstView d_v_labels)
  set the active discrete variable labels in currentVariables
• StringMultiArrayConstView discrete_string_variable_labels () const
  return the active discrete variable labels from currentVariables
• void discrete_string_variable_labels (StringMultiArrayConstView d_v_labels)
  set the active discrete variable labels in currentVariables
• StringMultiArrayConstView discrete_real_variable_labels () const
  return the active discrete variable labels from currentVariables
• void **discrete_real_variable_labels** (StringMultiArrayConstView d_v_labels)
  set the active discrete variable labels in currentVariables
• StringMultiArrayConstView **inactive_continuous_variable_labels** () const
  return the inactive continuous variable labels in currentVariables
• void **inactive_continuous_variable_labels** (StringMultiArrayConstView i_c_v_labels)
  set the inactive continuous variable labels in currentVariables
• StringMultiArrayConstView **inactive_discrete_int_variable_labels** () const
  return the inactive discrete variable labels in currentVariables
• void **inactive_discrete_int_variable_labels** (StringMultiArrayConstView i_d_v_labels)
  set the inactive discrete variable labels in currentVariables
• StringMultiArrayConstView **inactive_discrete_string_variable_labels** () const
  return the inactive discrete variable labels in currentVariables
• void **inactive_discrete_string_variable_labels** (StringMultiArrayConstView i_d_v_labels)
  set the inactive discrete variable labels in currentVariables
• StringMultiArrayConstView **inactive_discrete_real_variable_labels** () const
  return the inactive discrete variable labels in currentVariables
• void **inactive_discrete_real_variable_labels** (StringMultiArrayConstView i_d_v_labels)
  set the inactive discrete variable labels in currentVariables
• StringMultiArrayConstView **all_continuous_variable_labels** () const
  return all continuous variable labels in currentVariables
• void **all_continuous_variable_labels** (StringMultiArrayConstView a_c_v_labels)
  set all continuous variable labels in currentVariables
• void **all_continuous_variable_label** (const String &a_c_v_label, size_t i)
  set a label within the all continuous labels in currentVariables
• StringMultiArrayConstView **all_discrete_int_variable_labels** () const
  return all discrete variable labels in currentVariables
• void **all_discrete_int_variable_labels** (StringMultiArrayConstView a_d_v_labels)
  set all discrete variable labels in currentVariables
• void **all_discrete_int_variable_label** (const String &a_d_v_label, size_t i)
  set a label within the all discrete labels in currentVariables
• StringMultiArrayConstView **all_discrete_string_variable_labels** () const
  return all discrete variable labels in currentVariables
• void **all_discrete_string_variable_labels** (StringMultiArrayConstView a_d_v_labels)
  set all discrete variable labels in currentVariables
• void **all_discrete_string_variable_label** (const String &a_d_v_label, size_t i)
  set a label within the all discrete labels in currentVariables
• StringMultiArrayConstView **all_discrete_real_variable_labels** () const
  return all discrete variable labels in currentVariables
• void **all_discrete_real_variable_labels** (StringMultiArrayConstView a_d_v_labels)
  set all discrete variable labels in currentVariables
• void **all_discrete_real_variable_label** (const String &a_d_v_label, size_t i)
  set a label within the all discrete labels in currentVariables
• const StringArray & **response_labels** () const
return the response labels from currentResponse

- void response_labels (const StringArray &resp_labels)
  set the response labels in currentResponse

- const RealVector & continuous_lower_bounds () const
  return the active continuous lower bounds from userDefinedConstraints

- Real continuous_lower_bound (size_t i) const
  return an active continuous lower bound from userDefinedConstraints

- void continuous_lower_bounds (const RealVector &c_l_bnds)
  set the active continuous lower bounds in userDefinedConstraints

- void continuous_lower_bound (Real c_l_bnd, size_t i)
  set the i-th active continuous lower bound in userDefinedConstraints

- const RealVector & continuous_upper_bounds () const
  return the active continuous upper bounds from userDefinedConstraints

- Real continuous_upper_bound (size_t i) const
  return an active continuous upper bound from userDefinedConstraints

- void continuous_upper_bounds (const RealVector &c_u_bnds)
  set the active continuous upper bounds in userDefinedConstraints

- void continuous_upper_bound (Real c_u_bnd, size_t i)
  set the i-th active continuous upper bound in userDefinedConstraints

- const IntVector & discrete_int_lower_bounds () const
  return the active discrete int lower bounds from userDefinedConstraints

- int discrete_int_lower_bound (size_t i) const
  return an active discrete int lower bound from userDefinedConstraints

- void discrete_int_lower_bounds (const IntVector &d_l_bnds)
  set the active discrete int lower bounds in userDefinedConstraints

- void discrete_int_lower_bound (int d_l_bnd, size_t i)
  set the i-th active discrete int lower bound in userDefinedConstraints

- const IntVector & discrete_int_upper_bounds () const
  return the active discrete int upper bounds from userDefinedConstraints

- int discrete_int_upper_bound (size_t i) const
  return an active discrete int upper bound from userDefinedConstraints

- void discrete_int_upper_bounds (const IntVector &d_u_bnds)
  set the active discrete int upper bounds in userDefinedConstraints

- void discrete_int_upper_bound (int d_u_bnd, size_t i)
  set the i-th active discrete int upper bound in userDefinedConstraints

- const RealVector & discrete_real_lower_bounds () const
  return the active discrete real lower bounds from userDefinedConstraints

- Real discrete_real_lower_bound (size_t i) const
  return an active discrete real lower bound from userDefinedConstraints

- void discrete_real_lower_bounds (const RealVector &d_l_bnds)
  set the active discrete real lower bounds in userDefinedConstraints

- void discrete_real_lower_bound (Real d_l_bnd, size_t i)
  set the i-th active discrete real lower bound in userDefinedConstraints
• const RealVector & discrete_real_upper_bounds () const
  return the active discrete real upper bounds from userDefinedConstraints
• Real discrete_real_upper_bound (size_t i) const
  return an active discrete real upper bound from userDefinedConstraints
• void discrete_real_upper_bounds (const RealVector &d_u_bnds)
  set the active discrete real upper bounds in userDefinedConstraints
• void discrete_real_upper_bound (Real d_u_bnd, size_t i)
  set the i-th active discrete real upper bound in userDefinedConstraints
• const RealVector & inactive_continuous_lower_bounds () const
  return the inactive continuous lower bounds in userDefinedConstraints
• void inactive_continuous_lower_bounds (const RealVector &i_c_l_bnds)
  set the inactive continuous lower bounds in userDefinedConstraints
• const RealVector & inactive_continuous_upper_bounds () const
  return the inactive continuous upper bounds in userDefinedConstraints
• void inactive_continuous_upper_bounds (const RealVector &i_c_u_bnds)
  set the inactive continuous upper bounds in userDefinedConstraints
• const IntVector & inactive_discrete_int_lower_bounds () const
  return the inactive discrete lower bounds in userDefinedConstraints
• void inactive_discrete_int_lower_bounds (const IntVector &i_d_l_bnds)
  set the inactive discrete lower bounds in userDefinedConstraints
• const IntVector & inactive_discrete_int_upper_bounds () const
  return the inactive discrete upper bounds in userDefinedConstraints
• void inactive_discrete_int_upper_bounds (const IntVector &i_d_u_bnds)
  set the inactive discrete upper bounds in userDefinedConstraints
• const RealVector & inactive_discrete_real_lower_bounds () const
  return the inactive discrete lower bounds in userDefinedConstraints
• void inactive_discrete_real_lower_bounds (const RealVector &i_d_l_bnds)
  set the inactive discrete lower bounds in userDefinedConstraints
• const RealVector & inactive_discrete_real_upper_bounds () const
  return the inactive discrete upper bounds in userDefinedConstraints
• void inactive_discrete_real_upper_bounds (const RealVector &i_d_u_bnds)
  set the inactive discrete upper bounds in userDefinedConstraints
• const RealVector & all_continuous_lower_bounds () const
  return all continuous lower bounds in userDefinedConstraints
• void all_continuous_lower_bounds (const RealVector &a_c_l_bnds)
  set all continuous lower bounds in userDefinedConstraints
• void all_continuous_lower_bound (Real a_c_l_bnd, size_t i)
  set a lower bound within continuous lower bounds in userDefinedConstraints
• const RealVector & all_continuous_upper_bounds () const
  return all continuous upper bounds in userDefinedConstraints
• void all_continuous_upper_bounds (const RealVector &a_c_u_bnds)
  set all continuous upper bounds in userDefinedConstraints
• void all_continuous_upper_bound (Real a_c_u_bnd, size_t i)
set an upper bound within all continuous upper bounds in userDefinedConstraints

- const IntVector & all_discrete_int_lower_bounds () const
  return all discrete lower bounds in userDefinedConstraints
- void all_discrete_int_lower_bounds (const IntVector &a_d_l_bnds)
  set all discrete lower bounds in userDefinedConstraints
- void all_discrete_int_upper_bound (int a_d_u_bnd, size_t i)
  set a lower bound within all discrete lower bounds in userDefinedConstraints
- const IntVector & all_discrete_int_upper_bounds () const
  return all discrete upper bounds in userDefinedConstraints
- void all_discrete_int_upper_bounds (const IntVector &a_d_u_bnds)
  set all discrete upper bounds in userDefinedConstraints
- void all_discrete_int_upper_bound (int a_d_u_bnd, size_t i)
  set an upper bound within all discrete upper bounds in userDefinedConstraints
- const RealVector & all_discrete_real_lower_bounds () const
  return all discrete lower bounds in userDefinedConstraints
- void all_discrete_real_lower_bounds (const RealVector &a_d_l_bnds)
  set all discrete lower bounds in userDefinedConstraints
- void all_discrete_real_lower_bound (Real a_d_l_bnd, size_t i)
  set a lower bound within all discrete lower bounds in userDefinedConstraints
- const RealVector & all_discrete_real_upper_bounds () const
  return all discrete upper bounds in userDefinedConstraints
- void all_discrete_real_upper_bounds (const RealVector &a_d_u_bnds)
  set all discrete upper bounds in userDefinedConstraints
- void all_discrete_real_upper_bound (Real a_d_u_bnd, size_t i)
  set an upper bound within all discrete upper bounds in userDefinedConstraints
- size_t num_linear_ineq_constraints () const
  return the number of linear inequality constraints
- size_t num_linear_eq_constraints () const
  return the number of linear equality constraints
- const RealMatrix & linear_ineq_constraint_coeffs () const
  return the linear inequality constraint coefficients
- void linear_ineq_constraint_coeffs (const RealMatrix &lin_ineq_coeffs)
  set the linear inequality constraint coefficients
- const RealVector & linear_ineq_constraint_lower_bounds () const
  return the linear inequality constraint lower bounds
- void linear_ineq_constraint_lower_bounds (const RealVector &lin_ineq_l_bnds)
  set the linear inequality constraint lower bounds
- const RealVector & linear_ineq_constraint_upper_bounds () const
  return the linear inequality constraint upper bounds
- void linear_ineq_constraint_upper_bounds (const RealVector &lin_ineq_u_bnds)
  set the linear inequality constraint upper bounds
- const RealMatrix & linear_eq_constraint_coeffs () const
  return the linear equality constraint coefficients
• void linear_eq_constraint_coeffs (const RealMatrix &lin_eq_coeffs)
  set the linear equality constraint coefficients
• const RealVector & linear_eq_constraint_targets () const
  return the linear equality constraint targets
• void linear_eq_constraint_targets (const RealVector &lin_eq_targets)
  set the linear equality constraint targets
• size_t num_nonlinear_ineq_constraints () const
  return the number of nonlinear inequality constraints
• size_t num_nonlinear_eq_constraints () const
  return the number of nonlinear equality constraints
• const RealVector & nonlinear_ineq_constraint_lower_bounds () const
  return the nonlinear inequality constraint lower bounds
• void nonlinear_ineq_constraint_lower_bounds (const RealVector &nln_ineq_l_bnds)
  set the nonlinear inequality constraint lower bounds
• const RealVector & nonlinear_ineq_constraint_upper_bounds () const
  return the nonlinear inequality constraint upper bounds
• void nonlinear_ineq_constraint_upper_bounds (const RealVector &nln_ineq_u_bnds)
  set the nonlinear inequality constraint upper bounds
• const RealVector & nonlinear_eq_constraint_targets () const
  return the nonlinear equality constraint targets
• void nonlinear_eq_constraint_targets (const RealVector &nln_eq_targets)
  set the nonlinear equality constraint targets
• const Variables & current_variables () const
  return the current variables (currentVariables) as const reference (preferred)
• Variables & current_variables ()
  return the current variables (currentVariables) in mutable form (special cases)
• const Constraints & user_defined_constraints () const
  return the user-defined constraints (userDefinedConstraints)
• const Response & current_response () const
  return the current response (currentResponse)
• ProblemDescDB & problem_description_db () const
  return the problem description database (probDescDB)
• ParallelLibrary & parallel_library () const
  return the parallel library (parallelLib)
• const String & model_type () const
  return the model type (modelType)
• const String & surrogate_type () const
  return the surrogate type (surrogateType)
• const String & model_id () const
  return the model identifier (modelId)
• size_t num_functions () const
  return number of functions in currentResponse
• size_t num_primary_fns () const
return number of primary functions (total less nonlinear constraints)

- `size_t num_secondary_fns() const`
  return number of secondary functions (number of nonlinear constraints)

- `const String & gradient_type() const`
  return the gradient evaluation type (gradientType)

- `const String & method_source() const`
  return the numerical gradient evaluation method source (methodSource)

- `const String & interval_type() const`
  return the numerical gradient evaluation interval type (intervalType)

- `bool ignore_bounds() const`
  option for ignoring bounds when numerically estimating derivatives

- `bool central_hess() const`
  option for using old 2nd-order scheme when computing finite-diff Hessian

- `const RealVector & fd_gradient_step_size() const`
  return the finite difference gradient step size (fdGradStepSize)

- `const String & fd_gradient_step_type() const`
  return the finite difference gradient step type (fdGradStepType)

- `const IntSet & gradient_id_analytic() const`
  return the mixed gradient analytic IDs (gradIdAnalytic)

- `const IntSet & gradient_id_numerical() const`
  return the mixed gradient numerical IDs (gradIdNumerical)

- `const String & hessian_type() const`
  return the Hessian evaluation type (hessianType)

- `const String & quasi_hessian_type() const`
  return the Hessian evaluation type (quasiHessType)

- `const RealVector & fd_hessian_by_grad_step_size() const`
  return gradient-based finite difference Hessian step size (fdHessByGradStepSize)

- `const RealVector & fd_hessian_by_fn_step_size() const`
  return function-based finite difference Hessian step size (fdHessByFnStepSize)

- `const String & fd_hessian_step_type() const`
  return the finite difference Hessian step type (fdHessStepType)

- `const IntSet & hessian_id_analytic() const`
  return the mixed Hessian analytic IDs (hessIdAnalytic)

- `const IntSet & hessian_id_numerical() const`
  return the mixed Hessian analytic IDs (hessIdNumerical)

- `const IntSet & hessian_id_quasi() const`
  return the mixed Hessian analytic IDs (hessIdQuasi)

- `void primary_response_fn_sense(const BoolDeque & sense)`
  set the optimization sense for multiple objective functions

- `const BoolDeque & primary_response_fn_sense() const`
  get the optimization sense for multiple objective functions

- `const RealVector & primary_response_fn_weights() const`
  get the relative weightings for multiple objective functions or least squares terms
• const ScalingOptions & scaling_options () const
  user-provided scaling options
• short primary_fn_type () const
  get the primary response function type (generic, objective, calibration)
• void primary_fn_type (short type)
  set the primary response function type, e.g., when recasting
• bool derivative_estimation ()
  indicates potential usage of estimate_derivatives() based on gradientType/hessianType
• void supports_derivative_estimation (bool sed_flag)
  set whether this model should perform or pass on derivative estimation
• void init_comms_bcast_flag (bool icb_flag)
  set initCommsBcastFlag
• int evaluation_capacity () const
  return the evaluation capacity for use in iterator logic
• int derivative_concurrency () const
  return the gradient concurrency for use in parallel configuration logic
• bool asynch_flag () const
  return the asynchronous evaluation flag (asynchEvalFlag)
• void asynch_flag (const bool flag)
  set the asynchronous evaluation flag (asynchEvalFlag)
• short output_level () const
  return the outputLevel
• void output_level (const short level)
  set the outputLevel
• const IntArray & message_lengths () const
  return the array of MPI packed message buffer lengths (messageLengths)
• void parallel_configuration_iterator (ParConfigLIter pc_iter)
  set modelPCIter
• ParConfigLIter parallel_configuration_iterator () const
  return modelPCIter
• void auto_graphics (const bool flag)
  set modelAutoGraphicsFlag to activate posting of graphics data within evaluate/synchronize functions (automatic graphics posting in the model as opposed to graphics posting at the strategy level).
• bool is_null () const
  function to check modelRep (does this envelope contain a letter)
• Model * model_rep () const
  returns modelRep for access to derived class member functions that are not mapped to the top Model level
Static Public Member Functions

- static void active_variables (const RealVector &config_vars, Model &model)
  set the specified configuration to the Model’s inactive vars, converting from real to integer or through index to string value as needed

- static void inactive_variables (const RealVector &config_vars, Model &model)
  set the specified configuration to the Model’s inactive vars, converting from real to integer or through index to string value as needed

- static void inactive_variables (const RealVector &config_vars, Model &model, Variables &updated_vars)

Protected Member Functions

- Model (BaseConstructor, ProblemDescDB &problem_db)
  constructor initializing the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

- Model (LightWtBaseConstructor, ProblemDescDB &problem_db, ParallelLibrary &parallel_lib, const SharedVariablesData &svd, const SharedResponseData &srd, const ActiveSet &set, short output_level)
  constructor initializing base class for derived model class instances constructed on the fly

- Model (LightWtBaseConstructor, ProblemDescDB &problem_db, ParallelLibrary &parallel_lib)
  constructor initializing base class for recast model instances

- virtual void derived_evaluate (const ActiveSet &set)
  portion of evaluate() specific to derived model classes

- virtual void derived_evaluate_nowait (const ActiveSet &set)
  portion of evaluate_nowait() specific to derived model classes

- virtual const IntResponseMap & derived_synchronize ()
  portion of synchronize() specific to derived model classes

- virtual const IntResponseMap & derived_synchronize_nowait ()
  portion of synchronize_nowait() specific to derived model classes

- virtual void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  portion of init_communicators() specific to derived model classes

- virtual void derived_init_serial ()
  portion of init_serial() specific to derived model classes

- virtual void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  portion of set_communicators() specific to derived model classes

- virtual void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  portion of free_communicators() specific to derived model classes

- void set_ie_asynchronous_mode (int max_eval_concurrency)
  default logic for defining asynchEvalFlag and evaluationCapacity based on ie_pl settings

- void string_variable_max (const StringSetArray &ssa, size_t offset, Variables &vars)
  set the current value of each string variable offset + i to the longest string value found in the admissible string set ssa[i]

- void string_variable_max (const StringRealMapArray &srma, size_t offset, Variables &vars)
  set the current value of each string variable offset + i to the longest string value found in the admissible string map srma[i]
• SizetMultiArrayConstView initialize_x0_bounds (const SizetArray &original_dv, bool &active_derivs, bool &inactive_derivs, RealVector &x0, RealVector &fd_lb, RealVector &fd_ub) const
  Initialize data needed for computing finite differences (active/inactive, center point, and bounds)
• Real forward_grad_step (size_t num_deriv_vars, size_t xj_index, Real x0_j, Real lb_j, Real ub_j)
  Compute the forward step for a finite difference gradient; updates shortStep.
• template<typename MetaType>
  void rekey_response_map (MetaType &meta_object, const IntResponseMap &resp_map, IntIntMap &id_map, IntResponseMap &resp_map_rekey, bool deep_copy_resp=false)
  rekey returned jobs matched in id_map into resp_map_rekey; unmatched jobs are cached within the meta_object
• template<typename MetaType>
  void rekey_synch (MetaType &meta_object, bool block, IntIntMap &id_map, IntResponseMap &resp_map_rekey, bool deep_copy_resp=false)
  synchronize via meta_object and rekey returned jobs matched in id_map into resp_map_rekey; unmatched jobs are cached within the meta_object

Protected Attributes

• Variables currentVariables
  the set of current variables used by the model for performing function evaluations
• size_t numDerivVars
  the number of active continuous variables used in computing most response derivatives (i.e., in places such as quasi-Hessians and response corrections where only the active continuous variables are supported)
• Response currentResponse
  the set of current responses that holds the results of model function evaluations
• size_t numFns
  the number of functions in currentResponse
• Constraints userDefinedConstraints
  Explicit constraints on variables are maintained in the Constraints class hierarchy. Currently, this includes linear constraints and bounds, but could be extended in the future to include other explicit constraints which (1) have their form specified by the user, and (2) are not catalogued in Response since their form and coefficients are published to an iterator at startup.
• String modelId
  model identifier string from the input file
• String modelType
  type of model: simulation, nested, or surrogate
• String surrogateType
  type of surrogate model: local*, multipoint*, global*, or hierarchical
• String gradientType
  type of gradient data: analytic, numerical, mixed, or none
• String methodSource
  source of numerical gradient routine: dakota or vendor
• String intervalType
  type of numerical gradient interval: central or forward
• String hessianType
  type of Hessian data: analytic, numerical, quasi, mixed, or none
- RealVector \texttt{fdGradStepSize}
  relative finite difference step size for numerical gradients
- String \texttt{fdGradStepType}
  type of finite difference step to use for numerical gradient: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x
- RealVector \texttt{fdHessByGradStepSize}
  relative finite difference step size for numerical Hessians estimated using first-order differences of gradients
- RealVector \texttt{fdHessByFnStepSize}
  relative finite difference step size for numerical Hessians estimated using second-order differences of function values
- String \texttt{fdHessStepType}
  type of finite difference step to use for numerical Hessian: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x
- bool \texttt{ignoreBounds}
  option to ignore bounds when computing finite diffs
- bool \texttt{centralHess}
  option to use old 2nd-order finite diffs for Hessians
- bool \texttt{warmStartFlag}
  if in warm-start mode, don’t reset accumulated data (e.g., quasiHessians)
- bool \texttt{supportsEstimDerivs}
  whether model should perform or forward derivative estimation
- String \texttt{quasiHessType}
  quasi-Hessian type: bfgs, damped_bfgs, sr1
- IntSet \texttt{gradIdAnalytic}
  analytic id’s for mixed gradients
- IntSet \texttt{gradIdNumerical}
  numerical id’s for mixed gradients
- IntSet \texttt{hessIdAnalytic}
  analytic id’s for mixed Hessians
- IntSet \texttt{hessIdNumerical}
  numerical id’s for mixed Hessians
- IntSet \texttt{hessIdQuasi}
  quasi id’s for mixed Hessians
- IntArray \texttt{messageLengths}
  length of packed MPI buffers containing vars, vars/set, response, and PRPair
- ProblemDescDB & \texttt{probDescDB}
  class member reference to the problem description database
- ParallelLibrary & \texttt{parallelLib}
  class member reference to the parallel library
- ParConfigLIter \texttt{modelPCIter}
  the ParallelConfiguration node used by this Model instance
- short \texttt{componentParallelMode}
  the component parallelism mode: 0 (none), 1 (INTERFACE/OPTIONAL_INTERFACE/SURROGATE_MODEL), or 2 (SUB_MODEL/TRUTH_MODEL)
- bool \texttt{asynchEvalFlag}
flags asynch evaluations (local or distributed)

- int evaluationCapacity
  capacity for concurrent evaluations supported by the Model

- short outputLevel
  output verbosity level: \{SILENT, QUIET, NORMAL, VERBOSE, DEBUG\}, OUTPUT

- IntSetArray discreteDesignSetIntValues
  array of IntSet’s, each containing the set of allowable integer values corresponding to a discrete design integer set variable

- StringSetArray discreteDesignSetStringValues
  array of IntSet’s, each containing the set of allowable integer values corresponding to a discrete design string set variable

- RealSetArray discreteDesignSetRealValues
  array of RealSet’s, each containing the set of allowable real values corresponding to a discrete design real set variable

- IntSetArray discreteStateSetIntValues
  array of IntSet’s, each containing the set of allowable integer values corresponding to a discrete state integer set variable

- StringSetArray discreteStateSetStringValues
  array of IntSet’s, each containing the set of allowable integer values corresponding to a discrete state string set variable

- RealSetArray discreteStateSetRealValues
  array of RealSet’s, each containing the set of allowable real values corresponding to a discrete state real set variable

- Pecos::AleatoryDistParams aleatDistParams
  container for aleatory random variable distribution parameters

- Pecos::EpistemicDistParams epistDistParams
  container for epistemic random variable distribution parameters

- BoolDeque primaryRespFnSense
  array of flags (one per primary function) for switching the sense to maximize the primary function (default is minimize)

- RealVector primaryRespFnWts
  primary response function weightings (either weights for multiobjective optimization or weighted least squares)

- bool hierarchicalTagging
  whether to perform hierarchical evalID tagging of params/results

- ScalingOptions scalingOpts
  user-provided scaling data from the problem DB, possibly modified by Recasting

- String evalTagPrefix
  cached evalTag Prefix from parents to use at evaluate time

Private Member Functions

- Model * get_model (ProblemDescDB &problem_db)
  Used by the envelope to instantiate the correct letter class.

- int estimate_derivatives (const ShortArray &map_asv, const ShortArray &fd_grad_asv, const ShortArray &fd_hess_asv, const ShortArray &quasi_hess_asv, const ActiveSet &original_set, const bool asynch_flag)
evaluate numerical gradients using finite differences. This routine is selected with "method_source dakota" (the default method_source) in the numerical gradient specification.

- **void synchronize_derivatives** (const Variables &vars, const IntResponseMap &fd_responses, Response &new_response, const ShortArray &fd_grad_asv, const ShortArray &fd_hess_asv, const ShortArray &quasi_hess_asv, const ActiveSet &original_set)

    combine results from an array of finite difference response objects (fd_grad_responses) into a single response (new_response)

- **void update_response** (const Variables &vars, Response &new_response, const ShortArray &fd_grad_asv, const ShortArray &fd_hess_asv, const ShortArray &quasi_hess_asv, const ActiveSet &original_set, Response &initial_map_response, const RealMatrix &new_fn_grads, const RealSymMatrixArray &new_fn_hessians)

    overlay results to update a response object

- **void update_quasi_hessians** (const Variables &vars, Response &new_response, const ActiveSet &original_set)

    perform quasi-Newton Hessian updates

- **Real finite_difference_lower_bound** (UShortMultiArrayConstView cv_types, const RealVector &global_clbnds, size_t cv_index) const

    return the lower bound for a finite difference offset, drawn from global or distribution bounds

- **Real finite_difference_upper_bound** (UShortMultiArrayConstView cv_types, const RealVector &global_cu_bnds, size_t cv_index) const

    return the upper bound for a finite difference offset, drawn from global or distribution bounds

- **bool manage_asv** (const ActiveSet &original_set, ShortArray &map_asv_out, ShortArray &fd_grad_asv_out, ShortArray &fd_hess_asv_out, ShortArray &quasi_hess_asv_out)

    Coordinates usage of estimate_derivatives() calls based on asv_in.

- **Real initialize_h** (Real x_j, Real lb_j, Real ub_j, Real step_size, String step_type) const

    function to determine initial finite difference h (before step length adjustment) based on type of step desired

- **Real FDstep1** (Real x0_j, Real lb_j, Real ub_j, Real h_mag)

    function returning finite-difference step size (affected by bounds)

- **Real FDstep2** (Real x0_j, Real lb_j, Real ub_j, Real h)

    function returning second central-difference step size (affected by bounds)

### Private Attributes

- **int modelEvalCntr**

    evaluation counter for top-level evaluate() and evaluate_nowait() calls. Differs from lower level counters in case of numerical derivative estimation (several lower level evaluations are assimilated into a single higher level evaluation)

- **bool estDerivsFlag**

    flags presence of estimated derivatives within a set of calls to evaluate_nowait()

- **bool shortStep**

    flags finite-difference step size adjusted by bounds

- **std::map< SizetIntPair, ParConfigLIter > modelPCIterMap**

    map<> used for tracking modelPCIter instances using depth of parallelism level and max evaluation concurrency as the lookup keys

- **bool initCommsBcastFlag**
flag for determining need to broadcast the max concurrency from init_communicators(); set from IteratorScheduler::init_iterator()

- bool modelAutoGraphicsFlag
  flag for posting of graphics data within evaluate() (automatic graphics posting in the model as opposed to graphics posting at the strategy level)

- IntVariablesMap varsMap
  history of vars populated in evaluate_nowait() and used in synchronize().

- std::list<ShortArray> asvList
  if estimate_derivatives() is used, transfers ASVs from evaluate_nowait() to synchronize()

- std::list<ActiveSet> setList
  if estimate_derivatives() is used, transfers ActiveSets from evaluate_nowait() to synchronize()

- BoolList initialMapList
  transfers initial_map flag values from estimate_derivatives() to synchronize_derivatives()

- BoolList dbCaptureList
  transfers db_capture flag values from estimate_derivatives() to synchronize_derivatives()

- ResponseList dbResponseList
  transfers database captures from estimate_derivatives() to synchronize_derivatives()

- RealList deltaList
  transfers deltas from estimate_derivatives() to synchronize_derivatives()

- IntIntMap numFDEvalsMap
  tracks the number of evaluations used within estimate_derivatives(). Used in synchronize() as a key for combining finite difference responses into numerical gradients.

- IntIntMap rawEvalIdMap
  maps from the raw evaluation ids returned by derived_synchronize() and derived_synchronize_nowait() to the corresponding modelEvalCntr id. Used for rekeying responseMap.

- RealVectorArray xPrev
  previous parameter vectors used in computing s for quasi-Newton updates

- RealMatrix fnGradsPrev
  previous gradient vectors used in computing y for quasi-Newton updates

- RealSymMatrixArray quasiHessians
  quasi-Newton Hessian approximations

- SizetArray numQuasiUpdates
  number of quasi-Newton Hessian updates applied

- IntResponseMap responseMap
  used to return a map of responses for asynchronous evaluations in final concatenated form. The similar map in Interface contains raw responses.

- IntResponseMap cachedResponseMap
  caching of responses returned by derived_synchronize{,nowait}() but not matched within current rawEvalIdMap

- IntResponseMap graphicsRespMap
  used to cache the data returned from derived_synchronize_nowait() prior to sequential input into the graphics

- IntSetArray activeDiscSetIntValues
  aggregation of the admissible value sets for all active discrete set integer variables

- StringSetArray activeDiscSetStringValues
  aggregation of the admissible value sets for all active discrete set string variables
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- RealSetArray activeDiscSetRealValues
  aggregation of the admissible value sets for all active discrete set real variables
- BitArray discreteIntSets
  key for identifying discrete integer set variables within the active discrete integer variables
- ModelList modelList
  used to collect sub-models for subordinate_models()
- BoolDeque recastFlags
  a key indicating which models within a model recursion involve recasting
- Model * modelRep
  pointer to the letter (initialized only for the envelope)
- int referenceCount
  number of objects sharing modelRep

Friends

- bool operator==(const Model &m1, const Model &m2)
  equality operator (detect same letter instance)
- bool operator!=(const Model &m1, const Model &m2)
  inequality operator (detect different letter instances)

13.80.1 Detailed Description

Base class for the model class hierarchy.

The Model class is the base class for one of the primary class hierarchies in DAKOTA. The model hierarchy contains a set of variables, an interface, and a set of responses, and an iterator operates on the model to map the variables into responses using the interface. For memory efficiency and enhanced polymorphism, the model hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Model) serves as the envelope and one of the derived classes (selected in Model::get_model()) serves as the letter.

13.80.2 Constructor & Destructor Documentation

Model ( )

default constructor

The default constructor is used in vector<Model> instantiations and for initialization of Model objects contained in Iterator and derived Strategy classes. modelRep is NULL in this case (a populated problem_db is needed to build a meaningful Model object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

Model ( ProblemDescDB & problem_db )

standard constructor for envelope

Used in model instantiations within strategy constructors. Envelope constructor only needs to extract enough data to properly execute get_model, since Model(BaseConstructor, problem_db) builds the actual base class data for the derived models.

References Dakota::abort_handler(), Model::get_model(), and Model::modelRep.
13.80. MODEL CLASS REFERENCE

Model ( const Model & model )

copy constructor
  Copy constructor manages sharing of modelRep and incrementing of referenceCount.
  References Model::modelRep, and Model::referenceCount.

~Model ( ) [virtual]
destructor
  Destructor decrements referenceCount and only deletes modelRep when referenceCount reaches zero.
  References Model::modelRep, and Model::referenceCount.

Model ( BaseConstructor, ProblemDescDB & problem_db ) [protected]

constructor initializing the base class part of letter classes (BaseConstructor overloading avoids infinite recursion
in the derived class constructors - Coplien, p. 139)
  This constructor builds the base class data for all inherited models. get_model() instantiates a derived class
  and the derived class selects this base class constructor in its initialization list (to avoid the recursion of the base
  class constructor calling get_model() again). Since the letter IS the representation, its representation pointer is set
to NULL (an uninitialized pointer causes problems in ~Model).
  References Dakota::abort_handler(), Model::currentResponse, Model::fdGradStepSize, Model::fdHessByFn-
  StepSize, Model::fdHessByGradStepSize, ProblemDescDB::get_sa(), Model::gradIdNumerical, Model::gradient-
  Type, Model::hessianType, Model::hessIdNumerical, Response::num_functions(), Constraints::num_nonlinear_
  eq_constraints(), Constraints::num_nonlinear_ineq_constraints(), Model::primaryRespFnSense, Dakota::strbegins(),
  Dakota::strtolower(), and Model::userDefinedConstraints.

Model ( LightWtBaseConstructor, ProblemDescDB & problem_db, ParallelLibrary & parallel_lib ) [protected]

constructor initializing base class for recast model instances
  This constructor also builds the base class data for inherited models. However, it is used for recast models
  which are instantiated on the fly. Therefore it only initializes a small subset of attributes.

13.80.3 Member Function Documentation

Model operator= ( const Model & model )

assignment operator
  Assignment operator decrements referenceCount for old modelRep, assigns new modelRep, and increments
  referenceCount for new modelRep.
  References Model::modelRep, and Model::referenceCount.

Iterator & subordinate_iterator ( ) [virtual]

return the sub-iterator in nested and surrogate models
  return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this
  operation must be performed on the original envelope object.
  Reimplemented in RecastModel, DataFitSurrModel, and NestedModel.
  References Dakota::dummy_iterator, Model::modelRep, and Model::subordinate_iterator().
Referenced by NonDPolynomialChaos::append expansion(), NonDExpansion::compute expansion(), NonDExpansion::compute print_converged_results(), NonDExpansion::compute print_iteration_results(), SurrBasedGlobalMinimizer::core_run(), NonDExpansion::finalize_sets(), NonDGlobalReliability::get_best_sample(), NonDPolynomialChaos::increment_grid_from_order(), NonDPolynomialChaos::increment_sample_sequence(), NonDExpansion::increment_sets(), NonDPolynomialChaos::increment_specification_sequence(), NonDExpansion::increment_specification_sequence(), DOTOptimizer::initialize(), CONMINOptimizer::initialize(), NCSUOptimizer::initialize(), NLPLPPOptimizer::initialize(), NonDExpansion::initialize_expansion(), NonDExpansion::initialize_sets(), NonDStochCollocation::initialize_u_space_model(), NonDPolynomialChaos::initialize_u_space_model(), NonDExpansion::initialize_u_space_model(), NonDPolynomialChaos::multilevel_regression(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), DataFitSurrBasedLocalMinimizer::pre_run(), NonDExpansion::refine_expansion(), SOLBase::SOLBase(), Model::subordinate_iterator(), RecastModel::subordinate_iterator(), NonDStochCollocation::update_global(), and NonDQUESOBayesCalibration::update_model().

Model & subordinate_model( ) [virtual]
return a single sub-model defined from subModel in nested and recast models and truth_model() in surrogate
tools; used for a directed dive through model recursions that may bypass some components.

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this
operation must be performed on the original envelope object.
Reimplemented in RecastModel, NestedModel, and SurrogateModel.
References Dakota::dummy_model, Model::modelRep, and Model::subordinate_model().

Referenced by NonDGlobalReliability::expected_feasibility(), NonDGlobalReliability::expectedImprovement(),
SurrogateModel::force_rebuild(), AdaptedBasisModel::get_sub_model(), NonDExpansion::initialize_expansion(),
Minimizer::initialize_run(), NonDExpansion::initialize_u_space_model(), NonDGlobalReliability::optimize_gaussian_process(), Minimizer::original_model(), LeastSq::post_run(), COLINOptimizer::post_run(), Optimizer::primary_resp_reducer(), LeastSq::primaryRespWeighter(), LeastSq::print_results(), Model::subordinate_model(), DataFitSurrModel::update_global(), and LeastSq::weight_model().

Model & surrogate_model( ) [virtual]
return the active approximation sub-model in surrogate models

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this
operation must be performed on the original envelope object.
Reimplemented in RecastModel, DataFitSurrModel, and HierarchSurrModel.
References Dakota::dummy_model, Model::modelRep, and Model::surrogate_model().

Referenced by NonDAdaptiveSampling::calc_score_delta_y(), NonDAdaptiveSampling::calc_score_topo_avg_persistence(),
NonDAdaptiveSampling::calc_score_topo_alm_hybrid(), NonDAdaptiveSampling::calc_score_topo_alm_hybrid(),
NonDBayesCalibration::construct_mcmc_model(), NonDMultilevelSampling::control_variate_mc(),
SurrBasedGlobalMinimizer::core_run(), DataFitSurrBasedLocalMinimizer::DataFitSurrBasedLocalMinimizer(),
SurrBasedLocalMinimizer::find_approx_response(), NonDMultilevelSampling::lf_increment(),
NonDMultilevelSampling::multilevel_control_variate_mc_Qcorr(), NonDMultilevelSampling::multilevel_control_variate_mc_Ycorr(),
NonDMultilevelSampling::multilevel_mc_Qsum(), NonDMultilevelSampling::multilevel_mc_Ysum(), NonDAdaptiveSampling::output_round_data(), Model::surrogate_model(), and RecastModel::surrogate_model().

Model & truth_model( ) [virtual]
return the active truth sub-model in surrogate models

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this
operation must be performed on the original envelope object.
Reimplemented in RecastModel, DataFitSurrModel, and HierarchSurrModel.
References Dakota::dummy_model, Model::modelRep, and Model::truth_model().

Referenced by DataFitSurrBasedLocalMinimizer::build(), NonDMultilevelSampling::compute_error_estimates(), NonDMultilevelSampling::control_variate_mc(), SurrBasedGlobalMinimizer::core_run(), DataFitSurrBasedLocalMinimizer::DataFitSurrBasedLocalMinimizer(), HierarchSurrBasedLocalMinimizer::find_center_truth(), DataFitSurrBasedLocalMinimizer::find_center_truth(), HierarchSurrBasedLocalMinimizer::find_star_truth(), SurrBasedLocalMinimizer::find truth_response(), SurrogateModel::force_rebuild(), SurrBasedMinimizer::initialize_graphics(), NonDPolynomialChaos::multifidelity_expansion(), NonDMultilevelSampling::multilevel_control_variate_mc_Qcorr(), NonDMultilevelSampling::multilevel_control_variate_mc_Ycorr(), NonDMultilevelSampling::multilevel_mc_Qsum(), NonDMultilevelSampling::multilevel_mc_Ysum(), NonDPolynomialChaos::multilevel_regression(), NonDBayesCalibration::NonDBayesCalibration(), NonDLocalReliability::NonDLocalReliability(), DataFitSurrBasedLocalMinimizer::pre run(), SurrBasedMinimizer::print_results(), NonDMultilevelSampling::print_results(), NonDPolynomialChaos::print_results(), NonDMultilevelSampling::shared_increment(), SurrogateModel::subordinate_model(), SurrBasedGlobalMinimizer::SurrBasedGlobalMinimizer(), SurrBasedLocalMinimizer::SurrBasedLocalMinimizer(), Model::truth_model(), RecastModel::truth_model(), DataFitSurrBasedLocalMinimizer::verify(), and HierarchSurrBasedLocalMinimizer::verify().

```cpp
void update_from_subordinate_model ( size_t depth = std::numeric_limits<size_t>::max() )
[virtual]
```

propagate vars/labels/bounds/targets from the bottom up

used only for instantiate-on-the-fly model recursions (all RecastModel instantiations and alternate DataFitSurrModel instantiations). Simulation, Hierarchical, and Nested Models do not redefine the function since they do not support instantiate-on-the-fly. This means that the recursion will stop as soon as it encounters a Model that was instantiated normally, which is appropriate since ProblemDescDB-constructed Models use top-down information flow and do not require bottom-up updating.

Reimplemented in RecastModel, and DataFitSurrModel.
References Model::modelRep, and Model::update_from_subordinate_model().

Referenced by NonDGlobalInterval::core_run(), NonDLocalInterval::core_run(), NonDLocalReliability::initialize_class_data(), NonDExpansion::initialize_expansion(), LeastSq::initialize_run(), Optimizer::initialize_run(), EffGlobalMinimizer::minimize_surrogates_on_model(), NonDGlobalReliability::optimize_gaussian_process(), DataFitSurrModel::update_from_subordinate_model(), Model::update_from_subordinate_model(), and RecastModel::update_from_subordinate_model().

```cpp
Interface & derived_interface ( ) [virtual]
```

return the interface employed by the derived model class, if present: SimulationModel::userDefinedInterface, DataSurrModel::approxInterface, or NestedModel::optionalInterface

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.

Reimplemented in RecastModel, DataFitSurrModel, NestedModel, and SimulationModel.

References Model::derived_interface(), Dakota::dummy_interface, and Model::modelRep.

Referenced by SurrBasedGlobalMinimizer::core_run(), Model::derived_interface(), and RecastModel::derived_interface().

```cpp
size_t solution_levels ( ) const [virtual]
```

number of discrete levels within solution control (SimulationModel)

return the number of levels within a solution / discretization hierarchy.

Reimplemented in RecastModel, and SimulationModel.

References Model::modelRep, and Model::solution_levels().
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Referenced by NonDMultilevelSampling::compute_error_estimates(), NonDPolynomialChaos::multifidelity_expansion(), NonDMultilevelSampling::multilevel_control_variate_mc_Qcorr(), NonDMultilevelSampling::multilevel_control_variate_mc_Ycorr(), NonDMultilevelSampling::multilevel_mc_Qsum(), NonDMultilevelSampling::multilevel_mc_Ysum(), NonDPolynomialChaos::multilevel_regression(), NonDPolynomialChaos::print_results(), Model::solution_levels(), and RecastModel::solution_levels.

void solution_level_index(size_t index) [virtual]
activate a particular level within the solution level control and return the cost estimate (SimulationModel)
activate a particular level within a solution / discretization hierarchy and return the cost estimate.
Reimplemented in RecastModel, and SimulationModel.
References Dakota::abort_handler(), Model::modelRep, and Model::solution_level_index().
Referenced by HierarchSurrModel::build_approximation(), HierarchSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate_nowait(), Model::solution_level_index(), and RecastModel::solution_level_index().

short local_eval_synchronization() [virtual]
return derived model synchronization setting
SimulationModels and HierarchSurrModels redefine this virtual function.
A default value of "synchronous" prevents asynch local operations for:

• NestedModels: a subiterator can support message passing parallelism, but not asynch local.
• DataFitSurrModels: while asynch evals on approximations will work due to some added bookkeeping, avoiding them is preferable.

Reimplemented in RecastModel, NestedModel, and SimulationModel.
References Model::local_eval_synchronization(), and Model::modelRep.
Referenced by Model::init_serial(), RecastModel::local_eval_synchronization(), Model::local_eval_synchronization(), and Model::set_ie_asynchronous_mode().

int local_eval_concurrency() [virtual]
return derived model asynchronous evaluation concurrency
SimulationModels and HierarchSurrModels redefine this virtual function.
Reimplemented in RecastModel, NestedModel, and SimulationModel.
References Model::local_eval_concurrency(), and Model::modelRep.
Referenced by RecastModel::local_eval_concurrency(), Model::local_eval_concurrency(), and Model::set_ie_asynchronous_mode().

const String & interface_id() const [virtual]
return the interface identifier
return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.
Reimplemented in RecastModel, DataFitSurrModel, NestedModel, and SimulationModel.
References Dakota::dummy_interface, Interface::interface_id(), Model::interface_id(), and Model::modelRep.
Referenced by NonDQUESTOBayesCalibration::aggregate_acceptance_chain(), NonDDREAMBayesCalibration::archive_acceptance_chain(), DataFitSurrBasedLocalMinimizer::build(), DataFitSurrModel::build_global(), DataFitSurrModel::DataFitSurrModel(), Model::db_lookup(), Model::estimate_message_lengths(), Model::evaluate(),
bool evaluation_cache ( bool recurse_flag = true ) const [virtual]

Indicates the usage of an evaluation cache by the Model.
Only Models including ApplicationInterfaces support an evaluation cache: surrogate, nested, and recast mappings are not stored in the cache. Possible exceptions: HierarchSurrModel, NestedModel::optionalInterface.
Reimplemented in RecastModel, DataFitSurrModel, and SimulationModel.
References Model::evaluation_cache(), and Model::modelRep.
Referenced by DataFitSurrModel::DataFitSurrModel(), DataFitSurrModel::evaluation_cache(), RecastModel::evaluation_cache(), Model::evaluation_cache(), DataFitSurrModel::import_points(), and Analyzer::read_variables_responses().

bool restart_file ( bool recurse_flag = true ) const [virtual]

Indicates the usage of a restart file by the Model.
Only Models including ApplicationInterfaces interact with the restart file: surrogate, nested, and recast mappings are not stored in restart. Possible exceptions: DataFitSurrModel::import_points(), NestedModel::optionalInterface.
Reimplemented in RecastModel, DataFitSurrModel, and SimulationModel.
References Model::modelRep, and Model::restart_file().
Referenced by DataFitSurrModel::import_points(), Analyzer::read_variables_responses(), DataFitSurrModel::restart_file(), RecastModel::restart_file(), and Model::restart_file().

void eval_tag_prefix ( const String & eval_id_str ) [virtual]

set the hierarchical eval ID tag prefix
Derived classes containing additional models or interfaces should implement this function to pass along to their sub Models/Interfaces.
Reimplemented in RecastModel, and SimulationModel.
References Model::eval_tag_prefix(), Model::evalTagPrefix, and Model::modelRep.
Referenced by HierarchSurrModel::build_approximation(), HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate_nowait(), DataFitSurrModel::derived_evaluate_nowait(), Iterator::eval_tag_prefix(), RecastModel::eval_tag_prefix(), and Model::eval_tag_prefix().

ModelList & subordinate_models ( bool recurse_flag = true )
return the sub-models in nested and surrogate models
since modelList is built with list insertions (using envelope copies), these models may not be used for model::assign_rep() since this operation must be performed on the original envelope object. They may, however, be used for letter-based operations (including assign_rep() on letter contents such as an interface).
References Model::derived_subordinate_models(), Model::modelList, Model::modelRep, and Model::subordinate_models().
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Referenced by DataFitSurrBasedLocalMinimizer::DataFitSurrBasedLocalMinimizer(), HierarchSurrBasedLocalMinimizer::HierarchSurrBasedLocalMinimizer(), DOTOptimizer::initialize(), CONMINOptimizer::initialize(), NCSUOptimizer::initialize(), NLPQLPOptimizer::initialize(), Model::manage_data_recastings(), NonDPolynomialChaos::multifidelity_expansion(), NonDExpansion::multifidelity_expansion(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), NonDMultilevelSampling::NonDMultilevelSampling(), SOLBase::SOLBase(), and Model::subordinate_models().

```cpp
void init_communicators ( ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag = true )
```

allocate communicator partitions for a model and store configuration in modelPCIterMap

The `init_communicators()` and derived `init_communicators()` functions are structured to avoid performing the messageLengths estimation more than once. `init_communicators()` (not virtual) performs the estimation and then forwards the results to derived `init_communicators` (virtual) which uses the data in different contexts.

References ParallelLibrary::bcast(), Model::derived_init_communicators(), Model::estimate_message_lengths(), ParallelLibrary::increment_parallel_configuration(), Model::init_communicators(), Model::initCommsBcastFlag, Model::messageLengths, Model::modelPCIter, Model::modelPCIterMap, Model::modelRep, ParallelLibrary::parallel_configuration_iterator(), ParallelLibrary::parallel_level_index(), and Model::parallelLib.

Referenced by SurrBasedMinimizer::derived_init_communicators(), NonDGlobalReliability::derived_init_communicators(), NonDLocalInterval::derived_init_communicators(), NonDExpansion::derived_init_communicators(), NonDGlobalInterval::derived_init_communicators(), NonDAdaptImpSampling::derived_init_communicators(), NonDGPImpSampling::derived_init_communicators(), NonDAdaptiveSampling::derived_init_communicators(), NonDLocalReliability::derived_init_communicators(), AdaptedBasisModel::derived_init_communicators(), NonDAdaptImpSampling::derived_init_communicators(), NonDGlobalReliability::derived_init_communicators(), ActiveSubspaceModel::derived_init_communicators(), AdaptedBasisModel::derived_init_communicators(), DataFitSurrModel::derived_init_communicators(), RecastModel::derived_init_communicators(), Iterator::derived_init_communicators(), DataFitSurrModel::derived_set_communicators(), Model::init_communicators(), and Model::serve_init_communicators().

```cpp
void init_serial ( )
```

for cases where `init_communicators()` will not be called, modify some default settings to behave properly in serial.

The `init_serial()` and derived `init_serial()` functions are structured to separate base class (common) operations from derived class (specialized) operations.

References Model::asynchEvalFlag, Model::derived_init_serial(), Model::init_serial(), Model::local_eval_synchronization(), and Model::modelRep.

Referenced by NestedModel::derived_init_serial(), HierarchSurrModel::derived_init_serial(), DataFitSurrModel::derived_init_serial(), RecastModel::derived_init_serial(), and Model::init_serial().

```cpp
void estimate_message_lengths ( )
```

estimate messageLengths for a model

This functionality has been pulled out of `init_communicators()` and defined separately so that it may be used in those cases when messageLengths is needed but model.init_communicators() is not called, e.g., for the master processor in the self-scheduling of a concurrent iterator strategy.

References Response::active_set_derivative_vector(), Model::aleatDistParams, Response::copy(), Variables::copy(), Model::currentResponse, Model::currentVariables, Variables::cv(), Model::discreteDesignSetStringValues, Model::discreteStateSetStringValues, Model::epistDistParams, Model::estimate_message_lengths(), Variables::icv(), Model::interface_id(), Model::messageLengths, Model::modelRep, ParallelLibrary::mpirun_flag(), Model::numFns, Model::parallelLib, MPIPackBuffer::reset(), MPIPackBuffer::size(), and Model::string_variable_max().
void assign_rep ( Model * model_rep, bool ref_count_incr = true )

replaces existing letter with a new one

Similar to the assignment operator, the assign_rep() function decrements referenceCount for the old modelRep and assigns the new modelRep. It is different in that it is used for publishing derived class letters to existing envelopes, as opposed to sharing representations among multiple envelopes (in particular, assign_rep is passed a letter object and operator= is passed an envelope object). Letter assignment supports two models as governed by ref_count_incr:

- ref_count_incr = true (default): the incoming letter belongs to another envelope. In this case, increment the reference count in the normal manner so that deallocation of the letter is handled properly.

- ref_count_incr = false: the incoming letter is instantiated on the fly and has no envelope. This case is modeled after get_model(): a letter is dynamically allocated using new and passed into assign_rep, the letter’s reference count is not incremented, and the letter is not remotely deleted (its memory management is passed over to the envelope).

References Dakota::abort_handler(), Model::model_rep(), Model::modelRep, and Model::referenceCount.

Referenced by ActiveSubspaceModel::build_surrogate(), NonDBayesCalibration::calibrate_to_hifi(), ActiveSubspaceModel::computeCrossValidationMetric(), NonDBayesCalibration::construct_map_optimizer(), NonDBayesCalibration::construct_mcmc_model(), EffGlobalMinimizer::EffGlobalMinimizer(), ActiveSubspaceModel::get_sub_model(), SurrBasedLocalMinimizer::initialize_sub_model(), NonDAdaptiveSampling::NonDAdaptiveSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDGPlmpSampling::NonDGPlmpSampling(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), NonDPolynomialChaos::NonDPolynomialChaos(), NonDStochCollocation::NonDStochCollocation(), Optimizer::reduce_model(), NonDPolynomialChaos::resize(), Minimizer::scale_model(), NonD::transform_model(), and LeastSq::weight_model().

int derivative_concurrency ( ) const

return the gradient concurrency for use in parallel configuration logic

This function assumes derivatives with respect to the active continuous variables. Therefore, concurrency with respect to the inactive continuous variables is not captured.

References Dakota::contains(), Model::derivative_concurrency(), Model::gradIdAnalytic, Model::gradientType, Model::hessianType, Model::hessIdNumerical, Model::intervalType, Model::methodSource, Model::modelRep, and Model::numDerivVars.
void active_variables ( const RealVector & config_vars, Model & model ) [static]

set the specified configuration to the Model’s inactive vars, converting from real to integer or through index to string value as needed

  config_vars consists of [continuous, integer, string, real].

  References Model::continuous_variables(), Model::current_variables(), Model::cv(), Model::discrete_int_variables(), Model::discrete_real_variables(), Model::discrete_set_string_values(), Variables::discrete_string_variable(), Model::div(), Model::drv(), Model::dsv(), Dakota::iround(), and Dakota::set_index_to_value().

void inactive_variables ( const RealVector & config_vars, Model & model ) [static]

set the specified configuration to the Model’s inactive vars, converting from real to integer or through index to string value as needed

  config_vars consists of [continuous, integer, string, real].

  References Model::current_variables().

  Referenced by NonDBayesCalibration::build_model_discrepancy(), NonDBayesCalibration::calibrate_to_hifi(), DataTransformModel::derived_evaluate(), DataTransformModel::derived_evaluate_nowait(), and NonDBayesCalibration::export_discrepancy().

void inactive_variables ( const RealVector & config_vars, Model & model, Variables & vars ) [static]

config_vars consists of [continuous, integer, string, real].

  References Model::current_variables(), Model::discrete_set_string_values(), Model::icv(), Model::idiv(), Model::idrv(), Model::idsv(), Variables::inactive_continuous_variables(), Variables::inactive_discrete_int_variables(), Variables::inactive_discrete_real_variables(), Variables::inactive_discrete_string_variable(), Dakota::iround(), Dakota::set_index_to_value(), and Variables::view().

Model * get_model ( ProblemDescDB & problem_db ) [private]

Used by the envelope to instantiate the correct letter class.

  Used only by the envelope constructor to initialize modelRep to the appropriate derived type, as given by the modelType attribute.

  References ProblemDescDB::get_string(), Model::model_type(), and Model::modelType.

  Referenced by Model::model().

int estimate_derivatives ( const ShortArray & map_asv, const ShortArray & fd_grad_asv, const ShortArray & fd_hess_asv, const ShortArray & quasi_hess_asv, const ActiveSet & original_set, const bool asynch_flag ) [private]

evaluate numerical gradients using finite differences. This routine is selected with "method_source dakota" (the default method_source) in the numerical gradient specification.

  Estimate derivatives by computing finite difference gradients, finite difference Hessians, and/or quasi-Newton Hessians. The total number of finite difference evaluations is returned for use by synchronize() to track response arrays, and it could be used to improve management of max_function_evaluations within the iterators. ! new logic
References Variables::all_continuous_variables(), Model::centralHess, Variables::continuous_variables(), Model::currentResponse, Model::currentVariables, Model::db_lookup(), Model::dbCaptureList, Model::dbResponseList, Model::deltaList, ActiveSet::derivative_vector(), Model::derived_evaluate(), Model::derived_evaluate_nowait(), Model::fdHessByFnStepSize, Model::fdHessByGradStepSize, Model::fdHessStepType, Model::FDstep1(), Model::FDstep2(), Dakota::find_index(), Model::forward_grad_step(), Response::function_gradients(), Response::function_values(), Model::ignoreBounds, Variables::inactive_continuous_variables(), Model::initialize_x0_bounds(), Model::initialMapList, Model::intervalType, Model::numFns, Model::outputLevel, ActiveSet::request_vector(), Response::shared_data(), Model::shortStep, and Model::update_response().

Referenced by Model::evaluate(), and Model::evaluate_nowait().

```cpp
void synchronize_derivatives ( const Variables & vars, const IntResponseMap & fd_responses, Response & new_response, const ShortArray & fd_grad_asv, const ShortArray & fd_hess_asv, const ShortArray & quasi_hess_asv, const ActiveSet & original_set ) [private]
```

combine results from an array of finite difference response objects (fd_grad_responses) into a single response (new_response)

Merge an array of fd_responses into a single new_response. This function is used both by synchronous evaluate() for the case of asynchronous estimate_derivatives() and by synchronize() for the case where one or more evaluate_nowait() calls have employed asynchronous estimate_derivatives().

References Model::acv(), Variables::all_continuous_variable_ids(), Model::centralHess, Variables::continuous_variable_ids(), Model::currentResponse, Model::currentVariables, Model::cv(), Model::dbCaptureList, Model::dbResponseList, Model::deltaList, ActiveSet::derivative_vector(), Dakota::find_index(), Response::function_gradients(), Response::function_values(), Model::icv(), Variables::inactive_continuous_variable_ids(), Model::initialize_x0_bounds(), Model::initialMapList, Model::intervalType, Model::numFns, Response::shared_data(), and Model::update_response().

Referenced by Model::evaluate(), and Model::synchronize().

```cpp
void update_response ( const Variables & vars, Response & new_response, const ShortArray & fd_grad_asv, const ShortArray & fd_hess_asv, const ShortArray & quasi_hess_asv, const ActiveSet & original_set, Response & initial_map_response, const RealMatrix & new_fn_grads, const RealSymMatrixArray & new_fn_hessians ) [private]
```

overlay results to update a response object

Overlay the initial_map_response with numerically estimated new_fn_grads and new_fn_hessians to populate new_response as governed by asv vectors. Quasi-Newton secant Hessian updates are also performed here, since this is where the gradient data needed for the updates is first consolidated. Convenience function used by estimate_derivatives() for the synchronous case and by synchronize_derivatives() for the asynchronous case.

References Response::active_set_request_vector(), Variables::continuous_variable_ids(), Response::copy(), Model::currentResponse, Model::currentVariables, ActiveSet::derivative_vector(), Response::function_gradients(), Response::function_values(), Model::hessianType, Model::hessIdQuasi, Response::is_null(), Model::numFns, Model::outputLevel, Model::quasiHessians, ActiveSet::request_vector(), Response::reset_inactive(), Model::supportsEstimDerivs, Model::surrogate_response_mode(), and Model::update_quasi_hessians().

Referenced by Model::estimate_derivatives(), and Model::synchronize_derivatives().

```cpp
void update_quasi_hessians ( const Variables & vars, Response & new_response, const ActiveSet & original_set ) [private]
```

perform quasi-Newton Hessian updates

Quasi-Newton updates are performed for approximating response function Hessians using BFGS or SR1 formulations. These Hessians are supported only for the active continuous variables, and a check is performed on the DVV prior to invoking the function.
CHAPTER 13. CLASS DOCUMENTATION

References Dakota::contains(), Variables::continuous_variables(), Dakota::copy_data(), Model::fnGradsPrev, Response::function_gradients(), Model::hessianType, Model::hessIdQuasi, Model::modelType, Model::numDerivVars, Model::numFns, Model::numQuasiUpdates, Model::outputLevel, Model::quasiHessians, Model::quasiHessType, ActiveSet::request_vector(), and Model::xPrev.

Referenced by Model::update_response().

bool manage_asv ( const ActiveSet & original_set, ShortArray & map_asv_out, ShortArray & fd_grad_asv_out, ShortArray & fd_hess_asv_out, ShortArray & quasi_hess_asv_out ) [private]

Coordinates usage of estimate_derivatives() calls based on asv_in.

Splits asv_in total request into map_asv_out, fd_grad_asv_out, fd_hess_asv_out, and quasi_hess_asv_out as governed by the responses specification. If the returned use_est_deriv is true, then these asv outputs are used by estimate_derivatives() for the initial map, finite difference gradient evals, finite difference Hessian evals, and quasi-Hessian updates, respectively. If the returned use_est_deriv is false, then only map_asv_out is used.

References Dakota::abort_handler(), Dakota::contains(), ActiveSet::derivative_vector(), Model::FDstep2(), Dakota::find_index(), Model::forward_grad_step(), Model::gradIdAnalytic, Model::gradIdNumerical, Model::gradientType, Model::hessianType, Model::hessIdAnalytic, Model::hessIdNumerical, Model::hessIdQuasi, Model::ignoreBounds, Model::initialize_x0bounds(), Model::intervalType, Model::methodSource, ActiveSet::request_vector(), Model::shortStep, Model::supportsEstimDerivs, and Model::surrogate_response_mode().

Referenced by Model::evaluate(), and Model::evaluate_nowait().

Real initialize_h ( Real x_j, Real lb_j, Real ub_j, Real step_size, String step_type ) const [private]

function to determine initial finite difference h (before step length adjustment) based on type of step desired

Auxiliary function to determine initial finite difference h (before step length adjustment) based on type of step desired.

Referenced by Model::estimate_derivatives(), and Model::forward_grad_step().

Real FDstep1 ( Real x0_j, Real lb_j, Real ub_j, Real h_mag ) [private]

function returning finite-difference step size (affected by bounds)

Auxiliary function to compute forward or first central-difference step size, honoring bounds. The first step is away from zero, when possible. Flips the direction or updates shortStep if can’t take the full requested step h_mag.

References Model::ignoreBounds, and Model::shortStep.

Referenced by Model::estimate_derivatives(), and Model::forward_grad_step().

Real FDstep2 ( Real x0_j, Real lb_j, Real ub_j, Real h ) [private]

function returning second central-difference step size (affected by bounds)

Auxiliary function to compute the second central-difference step size, honoring bounds.

References Model::ignoreBounds, and Model::shortStep.

Referenced by Model::estimate_derivatives(), and Model::manage_asv().

13.80.4 Member Data Documentation

RealVector fdGradStepSize [protected]

relative finite difference step size for numerical gradients

A scalar value (instead of the vector fd_gradient_step_size spec) is used within the iterator hierarchy since this attribute is only used to publish a step size to vendor numerical gradient algorithms.
13.81. MPIManager Class Reference

Class MPIManager to manage Dakota’s MPI world, which may be a subset of MPI_COMM_WORLD.

Public Member Functions

- **MPIManager ()**
  
  *Default constructor; Dakota will not call MPI_Init.*

- **MPIManager (int &argc, char **&argv)**

  *Command-line constructor; parses MPI arguments during call to MPI_Init.*

- **MPIManager (MPI_Comm dakota mpi_comm)**

  *Construct on specified MPI_Comm.*

- **~MPIManager ()**

  *Destructor: calls finalize if Dakota owns MPI*

- **MPI_Comm dakota mpi_comm () const**
get the MPI Comm on which Dakota is running

- int world_rank() const
  get the rank of this process in Dakota’s MPI Comm

- int world_size() const
  get the size of the MPI Comm on which Dakota is running

- bool mpirun_flag() const
  true when Dakota is running in MPI mode

**Static Public Member Functions**

- static bool detect_parallel_launch(int argc, char **argv)
  detect parallel launch of Dakota using mpirun/mpiexec/poe/etc. based on command line arguments and environment variables

**Private Attributes**

- MPI Comm dakotaMPIComm
  MPI Comm on which DAKOTA is running.

- int dakotaWorldRank
  rank in MPI Comm in which DAKOTA is running

- int dakotaWorldSize
  size of MPI Comm in which DAKOTA is running

- bool mpirunFlag
  flag for a parallel mpirun/yod launch

- bool ownMPIFlag
  flag for ownership of MPI_Init/MPI_Finalize

### 13.81.1 Detailed Description

Class MPIManager to manage Dakota’s MPI world, which may be a subset of MPI_COMM_WORLD. The documentation for this class was generated from the following files:

- MPIManager.hpp
- MPIManager.cpp

### 13.82 MPIPackBuffer Class Reference

Class for packing MPI message buffers.

**Public Member Functions**

- MPIPackBuffer(int size = 1024)
  Constructor, which allows the default buffer size to be set.

- ~MPIPackBuffer()
  Destructor.

- const char *buf()
MPIPACKBUFFER CLASS REFERENCE

Returns a pointer to the internal buffer that has been packed.

- int size ()
  The number of bytes of packed data.
- int capacity ()
  the allocated size of Buffer.
- void reset ()
  Resets the buffer index in order to reuse the internal buffer.
- void pack (const int *data, const int num=1)
  Pack one or more int’s.
- void pack (const u_int *data, const int num=1)
  Pack one or more unsigned int’s.
- void pack (const long *data, const int num=1)
  Pack one or more long’s.
- void pack (const u_long *data, const int num=1)
  Pack one or more unsigned long’s.
- void pack (const short *data, const int num=1)
  Pack one or more short’s.
- void pack (const u_short *data, const int num=1)
  Pack one or more unsigned short’s.
- void pack (const char *data, const int num=1)
  Pack one or more char’s.
- void pack (const u_char *data, const int num=1)
  Pack one or more unsigned char’s.
- void pack (const double *data, const int num=1)
  Pack one or more double’s.
- void pack (const float *data, const int num=1)
  Pack one or more float’s.
- void pack (const bool *data, const int num=1)
  Pack one or more bool’s.
- void pack (const int &data)
  Pack a int.
- void pack (const u_int &data)
  Pack a unsigned int.
- void pack (const long &data)
  Pack a long.
- void pack (const u_long &data)
  Pack a unsigned long.
- void pack (const short &data)
  Pack a short.
- void pack (const u_short &data)
  Pack a unsigned short.
- void pack (const char &data)
  Pack a char.
CHAPTER 13. CLASS DOCUMENTATION

- void pack (const u_char &data)
  Pack a unsigned char.
- void pack (const double &data)
  Pack a double.
- void pack (const float &data)
  Pack a float.
- void pack (const bool &data)
  Pack a bool.

Protected Member Functions

- void resize (const int newsize)
  Resizes the internal buffer.

Protected Attributes

- char * Buffer
  The internal buffer for packing.
- int Index
  The index into the current buffer.
- int Size
  The total size that has been allocated for the buffer.

13.82.1 Detailed Description

Class for packing MPI message buffers.

A class that provides a facility for packing message buffers using the MPI_Pack facility. The MPIPackBuffer class dynamically resizes the internal buffer to contain enough memory to pack the entire object. When deleted, the MPIPackBuffer object deletes this internal buffer. This class is based on the Dakota_Version_3_0 version of utilib::PackBuffer from utilib/src/io/PackBuf.[cpp,h]

The documentation for this class was generated from the following files:

- MPIPackBuffer.hpp
- MPIPackBuffer.cpp

13.83 MPIUnpackBuffer Class Reference

Class for unpacking MPI message buffers.

Public Member Functions

- void setup (char *buf_, int size_, bool flag_=false)
  Method that does the setup for the constructors.
- MPIUnpackBuffer ()
  Default constructor.
- MPIUnpackBuffer (int size_)

Constructor that specifies the size of the buffer:

- **MPIUnpackBuffer** (char ∗buf, int size, bool flag=false)
  Constructor that sets the internal buffer to the given array.

- **~MPIUnpackBuffer** ()
  Destructor.

- **void resize** (const int newsize)
  Resizes the internal buffer.

- **const char ∗buf ()**
  Returns a pointer to the internal buffer.

- **int size ()**
  Returns the length of the buffer.

- **int curr ()**
  Returns the number of bytes that have been unpacked from the buffer.

- **void reset ()**
  Resets the index of the internal buffer.

- **void unpack** (int ∗data, const int num=1)
  Unpack one or more int’s.

- **void unpack** (u_int ∗data, const int num=1)
  Unpack one or more unsigned int’s.

- **void unpack** (long ∗data, const int num=1)
  Unpack one or more long’s.

- **void unpack** (u_long ∗data, const int num=1)
  Unpack one or more unsigned long’s.

- **void unpack** (short ∗data, const int num=1)
  Unpack one or more short’s.

- **void unpack** (u_short ∗data, const int num=1)
  Unpack one or more unsigned short’s.

- **void unpack** (char ∗data, const int num=1)
  Unpack one or more char’s.

- **void unpack** (u_char ∗data, const int num=1)
  Unpack one or more unsigned char’s.

- **void unpack** (double ∗data, const int num=1)
  Unpack one or more double’s.

- **void unpack** (float ∗data, const int num=1)
  Unpack one or more float’s.

- **void unpack** (bool ∗data, const int num=1)
  Unpack one or more bool’s.

- **void unpack** (int &data)
  Unpack a int.

- **void unpack** (u_int &data)
  Unpack a unsigned int.

- **void unpack** (long &data)
  Unpack a long.
• void unpack (u_long &data)
  Unpack a unsigned long.
• void unpack (short &data)
  Unpack a short.
• void unpack (u_short &data)
  Unpack a unsigned short.
• void unpack (char &data)
  Unpack a char.
• void unpack (u_char &data)
  Unpack a unsigned char.
• void unpack (double &data)
  Unpack a double.
• void unpack (float &data)
  Unpack a float.
• void unpack (bool &data)
  Unpack a bool.

Protected Attributes

• char * Buffer
  The internal buffer for unpacking.
• int Index
  The index into the current buffer.
• int Size
  The total size that has been allocated for the buffer.
• bool ownFlag
  If TRUE, then this class owns the internal buffer.

13.83.1 Detailed Description

Class for unpacking MPI message buffers.

A class that provides a facility for unpacking message buffers using the MPI_Unpack facility. This class is based on the Dakota_Version_3.0 version of utilib::UnPackBuffer from utilib/src/io/PackBuf.[cpp,h]

The documentation for this class was generated from the following files:

• MPIPackBuffer.hpp
• MPIPackBuffer.cpp

13.84 NCSUOptimizer Class Reference

Wrapper class for the NCSU DIRECT optimization library.

Inheritance diagram for NCSUOptimizer:
Public Member Functions

- `NCSUOptimizer (ProblemDescDB &problem_db, Model &model)`
  - standard constructor

- `NCSUOptimizer (Model &model, const int &max_iter, const int &max_eval, double min_box_size=-1.,
  double vol_box_size=-1., double solution_target=DBL_MAX)`
  - alternate constructor for instantiations "on the fly"

- `NCSUOptimizer (Model &model)`
  - alternate constructor for Iterator instantiations by name

- `NCSUOptimizer (const RealVector &var_lbnds, const RealVector &var_ubnds, const int &max_iter, const
  int &max_eval, double(*user_obj_eval)(const RealVector &x), double min_box_size=-1., double vol_box_-size=-1.,
  double solution_target=DBL_MAX)`
  - alternate constructor for instantiations "on the fly"

- `~NCSUOptimizer ()`
  - destructor

- `void core_run ()`
  - core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Private Member Functions

- `void initialize ()`
  - shared code among model-based constructors

- `void check_inputs ()`
  - verify problem respects NCSU DIRECT Fortran limits

Static Private Member Functions

- `static int objective_eval (int n, double c[ ], double l[ ], double u[ ], int point[ ], int *maxI, int *start, int
  *maxfunc, double fvec[ ], int idata[ ], int *isize, double ddata[ ], int *idsize, char cdata[ ], int *icsize)`
  - 'fep' in Griffin-modified NCSUDirect: computes the value of the objective function (potentially at multiple points,
  passed by function pointer to NCSUDirect). Include unscaling from DIRECT.
Private Attributes

- short **setUpType**
  controls iteration mode: **SETUP_MODEL** (normal usage) or **SETUP_USERFUNC** (user-supplied functions mode for "on the fly" instantiations). see enum in NCSUOptimizer.cpp **NonDGlobalReliability** currently uses the model mode. **GaussProcApproximation** currently uses the user functions mode.

- Real **minBoxSize**
  holds the minimum boxsize

- Real **volBoxSize**
  hold the minimum volume boxsize

- Real **solutionTarget**
  holds the solution target minimum to drive towards

- RealVector **lowerBounds**
  holds variable lower bounds passed in for "user functions" mode.

- RealVector **upperBounds**
  holds variable upper bounds passed in for "user functions" mode.

- double ( ∗ userObjectiveEval ) (const RealVector &x)
  holds function pointer for objective function evaluator passed in for "user functions" mode.

Static Private Attributes

- static NCSUOptimizer ∗ **ncsudirectInstance**
  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

13.84.1 Detailed Description

Wrapper class for the NCSU DIRECT optimization library.

The **NCSUOptimizer** class provides a wrapper for a Fortran 77 implementation of the DIRECT algorithm developed at North Carolina State University. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function or accessed through a static pointer.

The user input mappings are as follows:

13.84.2 Constructor & Destructor Documentation

NCSUOptimizer ( ProblemDescDB & *problem_db, Model & *model )

standard constructor

This is the standard constructor with method specification support.

References NCSUOptimizer::check_inputs(), and NCSUOptimizer::initialize().
NCSUOptimizer ( Model & model, const int & max_iter, const int & max_eval, double min_box_size = -1., double vol_box_size = -1., double solution_target = -DBL_MAX )

alternate constructor for instantiations "on the fly"

This is an alternate constructor for instantiations on the fly using a Model but no ProblemDescDB.
References NCSUOptimizer::check_inputs(), NCSUOptimizer::initialize(), Iterator::maxFunctionEvals, and Iterator::maxIterations.

NCSUOptimizer ( Model & model )

alternate constructor for Iterator instantiations by name

This is an alternate constructor for Iterator instantiations by name using a Model but no ProblemDescDB.
References NCSUOptimizer::check_inputs(), and NCSUOptimizer::initialize().

NCSUOptimizer ( const RealVector & var_lbnds, const RealVector & var_ubnds, const int & max_iter, const int & max_eval, double(*)(const RealVector &x) user_obj_eval, double min_box_size = -1., double vol_box_size = -1., double solution_target = -DBL_MAX )

alternate constructor for instantiations "on the fly"

This is an alternate constructor for performing an optimization using the passed in objective function pointer.
References NCSUOptimizer::check_inputs(), Iterator::maxFunctionEvals, and Iterator::maxIterations.

13.84.3 Member Function Documentation

void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
Reimplemented from Iterator.
References Dakota::abort_handler(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Iterator::convergenceTol, Dakota::copy_data(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, NCSUOptimizer::lowerBounds, Iterator::maxFunctionEvals, Iterator::maxIterations, NCSUOptimizer::minBoxSize, NCSUOptimizer::ncsudirectInstance, Minimizer::numContinuousVars, Minimizer::numFunctions, NCSUOptimizer::objective_eval(), Iterator::outputLevel, Model::primary_response_fn Sense(), NCSUOptimizer::setUpType, NCSUOptimizer::solutionTarget, NCSUOptimizer::upperBounds, and NCSUOptimizer::volBoxSize.

int objective_eval ( int * n, double c[], double l[], double u[], int point[], int * maxI, int * start, int * maxfunc, double fvec[], int iidata[], int * iisize, double ddata[], int * idsiz, char cdata[], int * icsize ) [static], [private]

'fep' in Griffin-modified NCSUDirect: computes the value of the objective function (potentially at multiple points, passed by function pointer to NCSUDirect). Include unscaling from DIRECT.
Modified batch evaluator that accepts multiple points and returns corresponding vector of functions in fvec. Must be used with modified DIRECT src (DIRbatch.f).
References Model::asynch_flag(), Model::continuous_variables(), Model::current_response(), Model::evaluate(), Model::evaluate_nowait(), Response::function_value(), Iterator::iteratedModel, NCSUOptimizer::ncsudirectInstance, Model::primary_response_fn Sense(), NCSUOptimizer::setUpType, Model::synchronize(), and NCSUOptimizer::userObjectiveEval.

Referenced by NCSUOptimizer::core_run().
The documentation for this class was generated from the following files:
13.85 NestedModel Class Reference

Derived model class which performs a complete sub-iterator execution within every evaluation of the model.

Inheritance diagram for NestedModel:

```
Model
  ↓
NestedModel
```

Public Member Functions

- **NestedModel (ProblemDescDB &problem_db)**
  constructor

- **~NestedModel ()**
  destructor

Protected Member Functions

- **void derived_evaluate (const ActiveSet &set)**
  portion of evaluate() specific to NestedModel

- **void derived_evaluate_nowait (const ActiveSet &set)**
  portion of evaluate_nowait() specific to NestedModel

- **const IntResponseMap & derived_synchronize ()**
  portion of synchronize() specific to NestedModel

- **Iterator & subordinate_iterator ()**
  return subIterator

- **Model & subordinate_model ()**
  return subModel

- **void derived_subordinate_models (ModelList &ml, bool recurse_flag)**
  return subModel

- **Interface & derived_interface ()**
  return optionalInterface

- **const RealVector & error_estimates ()**
  retrieve error estimates corresponding to the subIterator’s response results (e.g., statistical MSE for subordinate UQ).

- **void surrogate_response_mode (short mode)**
  pass a bypass request on to the subModel for any lower-level surrogates

- **void component_parallel_mode (short mode)**
  update component parallel mode for supporting parallelism in optionalInterface and subModel
• `size_t mi_parallel_level_index () const`
  
  `return subIteratorSched.miPLIndex`

• short `local_eval_synchronization ()`
  
  `return optionalInterface synchronization setting`

• int `local_eval_concurrency ()`
  
  `return optionalInterface asynchronous evaluation concurrency`

• bool `derived_master_overload () const`
  
  `flag which prevents overloading the master with a multiprocessor evaluation (forwarded to optionalInterface)`

• `IntIntPair estimate_partition_bounds (int max_eval_concurrency)`
  
  `estimate the minimum and maximum partition sizes that can be utilized by this Model`

• void `derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)`
  
  `set up optionalInterface and subModel for parallel operations`

• void `derived_init_serial ()`
  
  `set up optionalInterface and subModel for serial operations.

• void `derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)`
  
  `set active parallel configuration within subModel`

• void `derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)`
  
  `deallocate communicator partitions for the NestedModel (forwarded to optionalInterface and subModel)`

• void `serve_run (ParLevLIter pl_iter, int max_eval_concurrency)`
  
  `Service optionalInterface and subModel job requests received from the master. Completes when a termination message is received from stop_servers()).`

• void `stop_servers ()`
  
  `Executed by the master to terminate server operations for subModel and optionalInterface when iteration on the NestedModel is complete.`

• const String & `interface_id () const`
  
  `return the optionalInterface identifier`

• int `derived_evaluation_id () const`
  
  `Return the current evaluation id for the NestedModel.`

• void `set_evaluation_reference ()`
  
  `set the evaluation counter reference points for the NestedModel (request forwarded to optionalInterface and subModel)`

• void `fine_grained_evaluation_counters ()`
  
  `request fine-grained evaluation reporting within optionalInterface and subModel`

• void `print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const`
  
  `print the evaluation summary for the NestedModel (request forwarded to optionalInterface and subModel)`

• void `warm_start_flag (const bool flag)`
  
  `set the warm start flag, including actualModel`

• void `initialize_iterator (int job_index)`
  
  `void pack_parameters_buffer (MPIPackBuffer &send_buffer, int job_index)`

• void `unpack_parameters_buffer (MPIUnpackBuffer &recv_buffer, int job_index)`

• void `unpack_parameters_initialize (MPIUnpackBuffer &recv_buffer, int job_index)`

• void `pack_results_buffer (MPIPackBuffer &send_buffer, int job_index)`

• void `unpack_results_buffer (MPIUnpackBuffer &recv_buffer, int job_index)`

• void `update_local_results (int job_index)`
Private Member Functions

- void update_sub_iterator()
  - update sub_iterator with mapping data and set sub_iterator-based counts
- PRPQueueIter job_index_to_queue_iterator(int job_index)
  - convert job_index to an eval_id through subIteratorIdMap and eval_id to a subIteratorPRPQueue queue iterator
- void initialize_iterator(const Variables &vars, const ActiveSet &set, int eval_id)
  - lower level function shared by initialize_iterator(int) and unpack_parameters_initialize()
- void unpack(MPIUnpackBuffer &recv_buffer, int job_index, Variables &vars, ActiveSet &set, int &eval_id)
  - lower level function shared by unpack_parameters_buffer() and unpack_parameters_initialize()
- void resolve_real_variable_mapping(const String &map1, const String &map2, size_t curr_index, short &inactive_sm_view)
  - for a named real mapping, resolve primary index and secondary target
- void resolve_integer_variable_mapping(const String &map1, const String &map2, size_t curr_index, short &inactive_sm_view)
  - for a named integer mapping, resolve primary index and secondary target
- void resolve_string_variable_mapping(const String &map1, const String &map2, size_t curr_index, short &inactive_sm_view)
  - for a named string mapping, resolve primary index and secondary target
- size_t sm_acv_index_map(size_t pacvm_index, short sacvm_target)
  - offset pacvm_index based on sacvm_target to create mapped_index
- size_t sm_adiv_index_map(size_t padivm_index, short sadivm_target)
  - offset padivm_index based on sadivm_target to create mapped_index
- size_t sm_adsv_index_map(size_t padsvm_index, short sadsvm_target)
  - offset padsvm_index based on sadsvm_target to create mapped_index
- size_t sm_adrv_index_map(size_t padrvm_index, short sadrvm_target)
  - offset padrvm_index based on sadrvm_target to create mapped_index
- size_t cv_index_map(size_t cv_index, const Variables &vars)
  - offset cv_index to create index into aggregated primary/secondary arrays
- size_t div_index_map(size_t div_index, const Variables &vars)
  - offset div_index to create index into aggregated primary/secondary arrays
- size_t dsv_index_map(size_t dsv_index, const Variables &vars)
  - offset dsv_index to create index into aggregated primary/secondary arrays
- size_t drv_index_map(size_t drv_index, const Variables &vars)
  - offset drv_index to create index into aggregated primary/secondary arrays
- size_t ccv_index_map(size_t ccv_index, const Variables &vars)
  - offset active complement ccv_index to create index into all continuous arrays
- size_t cdv_index_map(size_t cdv_index, const Variables &vars)
  - offset active complement cdv_index to create index into all discrete int arrays
- size_t cdsv_index_map(size_t cdsv_index, const Variables &vars)
  - offset active complement cdsv_index to create index into all discrete string arrays
- size_t cdrv_index_map(size_t cdrv_index, const Variables &vars)
  - offset active complement cdrv_index to create index into all discrete real arrays
- void real_variable_mapping(const Real &r_var, size_t mapped_index, short svm_target)
insert r_var into appropriate recipient

• void integer_variable_mapping (const int &i_var, size_t mapped_index, short svm_target)
insert i_var into appropriate recipient

• void string_variable_mapping (const String &s_var, size_t mapped_index, short svm_target)
insert s_var into appropriate recipient

• void set_mapping (const ActiveSet &mapped_set, ActiveSet &interface_set, bool &opt_interface_map, ActiveSet &sub_iterator_set, bool &sub_iterator_map)
define the evaluation requirements for the optionalInterface (interface_set) and the subIterator (sub_iterator_set) from the total model evaluation requirements (mapped_set)

• void response_mapping (const Response &interface_response, const Response &sub_iterator_response, Response &mapped_response)
combine the response from the optional interface evaluation with the response from the sub-iteration using the primaryCoeffs/secondaryCoeffs mappings to create the total response for the model

• void interface_response_overlay (const Response &opt_interface_response, Response &mapped_response)
assign the response from the optional interface evaluation within the total response for the model

• void iterator_response_overlay (const Response &sub_iterator_response, Response &mapped_response)
overlay the sub-iteration response within the total response for the model using the primaryCoeffs/secondaryCoeffs mappings

• void iterator_error_estimation (const RealVector &sub_iterator_errors, RealVector &mapped_errors)
combine error estimates from the sub-iteration to define mappedErrorEstimates

• Response & nested_response (int nested_cntr)
locate existing or allocate new entry in nestedResponseMap

• void check_response_map (const ShortArray &mapped_asv)
check function counts for the mapped_asv

• void update_inactive_view (short new_view, short &view)
update inactive variables view for subIterator based on new_view

• void update_inactive_view (unsigned short type, short &view)
update inactive variables view for subIterator based on type

• void update_sub_model (const Variables &vars, const Constraints &cons)
update subModel with current variable values/bounds/labels

Private Attributes

• int nestedModelEvalCntr
number of calls to derived_evaluate()/derived_evaluate_nowait()

• bool firstUpdate
boolean to trigger one-time updates on first call to update_sub_model()

• IntResponseMap nestedResponseMap
used to return a map of nested responses (including subIterator and optionalInterface contributions) for aggregation and rekeying at the base class level

• RealVector mappedErrorEstimates
mapping of subIterator.response_error_estimates() through primary and secondary mappings

• size_t outerMIPLIndex
the miPLIndex for the outer parallelism context, prior to any subIterator partitioning

• Iterator subIterator
the sub-iterator that is executed on every evaluation of this model

- **String subMethodPointer**
  - the sub-method pointer from the nested model specification
- **Model subModel**
  - the sub-model used in sub-iterator evaluations
- **PRPQueue subIteratorPRPQueue**
  - job queue for asynchronous execution of subIterator jobs
- **IteratorScheduler subIteratorSched**
  - scheduling object for concurrent iterator parallelism
- **int subIteratorJobCntr**
  - subIterator job counter since last synchronize()
- **IntlIntMap subIteratorIdMap**
  - mapping from subIterator evaluation counter to nested model counter (different when subIterator evaluations do not occur on every nested model evaluation due to variable ASV content)
- **size_t numSubIterFns**
  - number of sub-iterator response functions prior to mapping
- **size_t numSubIterMappedIneqCon**
  - number of top-level inequality constraints mapped from the sub-iteration results
- **size_t numSubIterMappedEqCon**
  - number of top-level equality constraints mapped from the sub-iteration results
- **Interface optionalInterface**
  - the optional interface contributes nonnested response data to the total model response
- **String optInterfacePointer**
  - the optional interface pointer from the nested model specification
- **Response optInterfaceResponse**
  - the response object resulting from optional interface evaluations
- **IntlIntMap optInterfaceIdMap**
  - mapping from optionalInterface evaluation counter to nested model counter (different when optionalInterface evaluations do not occur on every nested model evaluation due to variable ASV content)
- **size_t numOptInterfPrimary**
  - number of primary response functions (objective/least squares/generic functions) resulting from optional interface evaluations
- **size_t numOptInterfIneqCon**
  - number of inequality constraints resulting from optional interface evaluations
- **size_t numOptInterfEqCon**
  - number of equality constraints resulting from the optional interface evaluations
- **SizetArray active1ACVarMapIndices**
  - "primary" variable mappings for inserting active continuous currentVariables within all continuous subModel variables. If there are no secondary mappings defined, then the insertions replace the subModel variable values.
- **SizetArray active1ADIVarMapIndices**
  - "primary" variable mappings for inserting active discrete int currentVariables within all discrete int subModel variables. No secondary mappings are defined for discrete int variables, so the active variables replace the subModel variable values.
- **SizetArray active1ADSVarMapIndices**
"primary" variable mappings for inserting active discrete string currentVariables within all discrete string sub-
Model variables. No secondary mappings are defined for discrete string variables, so the active variables replace
the subModel variable values.

- **SizetArray** active1ADRVarMapIndices
  "primary" variable mappings for inserting active discrete real currentVariables within all discrete real subModel
variables. No secondary mappings are defined for discrete real variables, so the active variables replace the sub-
Model variable values.

- **ShortArray** active2ACVarMapTargets
  "secondary" variable mappings for inserting active continuous currentVariables into sub-parameters (e.g., distri-
bution parameters for uncertain variables or bounds for continuous design/state variables) within all continuous
subModel variables.

- **ShortArray** active2ADIVarMapTargets
  "secondary" variable mappings for inserting active discrete int currentVariables into sub-parameters (e.g., bounds
for discrete design/state variables) within all discrete int subModel variables.

- **ShortArray** active2ADSVarMapTargets
  "secondary" variable mappings for inserting active discrete string currentVariables into sub-parameters (e.g.,
bounds for discrete design/state variables) within all discrete string subModel variables.

- **ShortArray** active2ADRVarMapTargets
  "secondary" variable mappings for inserting active discrete real currentVariables into sub-parameters (e.g., bounds
for discrete design/state variables) within all discrete real subModel variables.

- **SizetArray** complement1ACVarMapIndices
  "primary" variable mappings for inserting the complement of the active continuous currentVariables within all
continuous subModel variables

- **SizetArray** complement1ADIVarMapIndices
  "primary" variable mappings for inserting the complement of the active discrete int currentVariables within all
discrete int subModel variables

- **SizetArray** complement1ADSVarMapIndices
  "primary" variable mappings for inserting the complement of the active discrete string currentVariables within all
discrete string subModel variables

- **SizetArray** complement1ADRVarMapIndices
  "primary" variable mappings for inserting the complement of the active discrete real currentVariables within all
discrete real subModel variables

- **BitArray** extraCVarsData
  flags for updating subModel continuous bounds and labels, one for each active continuous variable in current-
Variables

- **BitArray** extraDIVarsData
  flags for updating subModel discrete int bounds and labels, one for each active discrete int variable in current-
Variables

- **BitArray** extraDSVarsData
  flags for updating subModel discrete string labels, one for each active discrete string variable in currentVariables

- **BitArray** extraDRVarsData
  flags for updating subModel discrete real bounds and labels, one for each active discrete real variable in current-
Variables

- **RealMatrix** primaryRespCoeffs
  "primary" response mapping matrix applied to the sub-iterator response functions. For OUU, the matrix is applied
to UQ statistics to create contributions to the top-level objective functions/least squares/ generic response terms.
• RealMatrix secondaryRespCoeffs

"secondary" response mapping matrix applied to the sub-iterator response functions. For OUU, the matrix is applied to UQ statistics to create contributions to the top-level inequality and equality constraints.

Friends
• class IteratorScheduler

protect scheduler callback functions from general access

Additional Inherited Members
13.85.1 Detailed Description
Derived model class which performs a complete sub-iterator execution within every evaluation of the model.

The NestedModel class nests a sub-iterator execution within every model evaluation. This capability is most commonly used for optimization under uncertainty, in which a nondeterministic iterator is executed on every optimization function evaluation. The NestedModel also contains an optional interface, for portions of the model evaluation which are independent from the sub-iterator, and a set of mappings for combining sub-iterator and optional interface data into a top level response for the model.

13.85.2 Member Function Documentation

void derived_evaluate ( const ActiveSet & set ) [protected], [virtual]

portion of evaluate() specific to NestedModel

Update subModel’s inactive variables with active variables from currentVariables, compute the optional interface and sub-iterator responses, and map these to the total model response.

Reimplemented from Model.

References NestedModel::active2ACVarMapTargets, Response::active_set(), ParallelLibrary::broadcast, ParallelLibrary::broadcast(), NestedModel::component_parallel_mode(), Model::currentResponse, Model::currentVariables, Interface::eval_tag_prefix(), Iterator::eval_tag_prefix(), Model::evalTagPrefix, Model::hierarchicalTagging, NestedModel::interface_response_overlay(), NestedModel::iterator_response_overlay(), IteratorScheduler::iteratorCommSize, IteratorScheduler::iteratorScheduling, Interface::map(), IteratorScheduler::messagePass, IteratorScheduler::mPLIndex, Model::modelPCIter, NestedModel::nestedModelEvalCntr, NestedModel::optInterfaceResponse, NestedModel::optionalInterfaceIdMap, NestedModel::optionalInterface, Iterator::response_results(), Iterator::response_results_active_set(), Iterator::run(), IteratorScheduler::run_iterator(), NestedModel::set_mapping(), IteratorScheduler::stop_iterator_servers(), NestedModel::subIterator, NestedModel::subIteratorSched, NestedModel::update_sub_model(), and Model::userDefinedConstraints.

void derived_evaluate_nowait ( const ActiveSet & set ) [protected], [virtual]

portion of evaluate_nowait() specific to NestedModel

Asynchronous execution of subIterator on subModel and, optionally, optionalInterface.

Reimplemented from Model.

References Response::active_set(), Model::currentResponse, Model::currentVariables, Interface::evaluation_id(), Interface::map(), Iterator::method_id(), NestedModel::nestedModelEvalCntr, NestedModel::optInterfaceIdMap, NestedModel::optInterfaceResponse, NestedModel::optionalInterface, Iterator::response_results(), Iterator::response_results_active_set(), NestedModel::set_mapping(), NestedModel::subIterator, NestedModel::subIteratorIdMap, NestedModel::subIteratorJobCntr, and NestedModel::subIteratorPRPQueue.
const IntResponseMap & derived synchronize() [protected], [virtual]

portion of synchronize() specific to NestedModel

Recovery of asynchronous subIterator executions and, optionally, asynchronous optionalInterface mappings.
Reimplemented from Model.

References Interface::cache_unmatched_response(), NestedModel::component_parallel_mode(), NestedModel-
::interface_response_overlay(), NestedModel::iterator_response_overlay(), Model::modelPCIter, NestedModel::nested-
_response(), NestedModel::nestedResponseMap, IteratorScheduler::numIteratorJobs, NestedModel::optInterface-
IdMap, NestedModel::optInterfacePointer, NestedModel::optionalInterface, ParallelLibrary::parallel_configuration-
 Iterator(), Model::parallelLib, IteratorScheduler::schedule_iterators(), NestedModel::subIterator, NestedModel-
::subIteratorIdMap, NestedModel::subIteratorJobCntr, NestedModel::subIteratorPRPQueue, NestedModel::sub-
IteratorSched, and Interface::synchronize().

short local_eval synchronization() [inline], [protected], [virtual]

return optionalInterface synchronization setting

Used in setting Model::asynchEvalFlag. subModel synchronization is used for setting asynchEvalFlag within
subModel.
Reimplemented from Model.
References Interface::asynch_local_evaluation_concurrency(), Interface::interface_synchronization(), Nested-
Model::optInterfacePointer, and NestedModel::optionalInterface.

int local_eval_concurrency() [inline], [protected], [virtual]

return optionalInterface asynchronous evaluation concurrency

Used in setting Model::evaluationCapacity. subModel concurrency is used for setting evaluationCapacity
within subModel.
Reimplemented from Model.
References Interface::asynch_local_evaluation_concurrency(), NestedModel::optInterfacePointer, and Nested-
Model::optionalInterface.

bool derived_master_overload() const [inline], [protected], [virtual]

flag which prevents overloading the master with a multiprocessor evaluation (forwarded to optionalInterface)

Derived master overload for subModel is handled separately in subModel.evaluate() within subIterator.run().
Reimplemented from Model.
References Iterator::is_null(), Interface::iterator_eval_dedicated_master(), IteratorScheduler::iteratorScheduling,
Interface::multi_proc_eval(), NestedModel::optInterfacePointer, NestedModel::optionalInterface, IteratorScheduler-
::procsPerIterator, NestedModel::subIterator, and NestedModel::subIteratorSched.

void derived_init_communicators( ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag =
true ) [protected], [virtual]

set up optionalInterface and subModel for parallel operations

Asynchronous flags need to be initialized for the subModel. In addition, max_eval_concurrency is the outer
level iterator concurrency, not the subIterator concurrency that subModel will see, and recomputing the message-
lengths on the subModel is probably not a bad idea either. Therefore, recompute everything on subModel using
init_communicators().
Reimplemented from Model.
References Response::active_set(), IteratorScheduler::configure(), Model::currentVariables, ProblemDescDB::get_db_method_node(), ProblemDescDB::get_db_model_node(), Interface::init_communicators(), IteratorScheduler::init_iterator(), Iterator::is_null(), IteratorScheduler::iterator_message_lengths(), IteratorScheduler::iteratorServerId, Model::messageLengths, IteratorScheduler::messagePass, Model::modelPCIter, IteratorScheduler::numIteratorServers, NestedModel::optInterfacePointer, NestedModel::optionalInterface, ParallelLibrary::parallel_configuration_iterator(), Model::parallelLib, IteratorScheduler::partition(), Model::probDescDB, MPIPackBuffer::reset(), Iterator::response_results(), ProblemDescDB::set_db_list_nodes(), ProblemDescDB::set_db_method_node(), ProblemDescDB::set_db_model_nodes(), MPIPackBuffer::size(), NestedModel::subIterator, NestedModel::subMethodPointer, NestedModel::subModel, IteratorScheduler::update(), and NestedModel::update_sub_iterator().

```cpp
int derived_evaluation_id ( ) const [inline], [protected], [virtual]
```

Return the current evaluation id for the NestedModel.

return the top level nested evaluation count. To get the lower level eval count, the subModel must be explicitly queried. This is consistent with the eval counter definitions in surrogate models.

Reimplemented from Model.

References NestedModel::nestedModelEvalCntr.

```cpp
size_t cv_index_map ( size_t cv_index, const Variables & vars ) [private]
```

offset cv_index to create index into aggregated primary/secondary arrays

maps index within active continuous variables to index within aggregated active continuous/discrete-int/discrete-string/discrete-real variables.

References SharedVariablesData::aleatory_uncertain_counts(), SharedVariablesData::design_counts(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().

```cpp
size_t div_index_map ( size_t div_index, const Variables & vars ) [private]
```

offset div_index to create index into aggregated primary/secondary arrays

maps index within active discrete int variables to index within aggregated active continuous/discrete-int/discrete-string/discrete-real variables.

References SharedVariablesData::aleatory_uncertain_counts(), Variables::cv(), SharedVariablesData::design_counts(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), SharedVariablesData::state_counts(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().

```cpp
size_t dsv_index_map ( size_t dsv_index, const Variables & vars ) [private]
```

offset dsv_index to create index into aggregated primary/secondary arrays

maps index within active discrete string variables to index within aggregated active continuous/discrete-int/discrete-string/discrete-string variables.

References SharedVariablesData::aleatory_uncertain_counts(), Variables::cv(), SharedVariablesData::design_counts(), Variables::div(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), SharedVariablesData::state_counts(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().
size_t drv_index_map (size_t drv_index, const Variables & vars) [private]

offset drv_index to create index into aggregated primary/secondary arrays
maps index within active discrete real variables to index within aggregated active continuous/discrete-int/discrete-string/discrete-real variables.

References SharedVariablesData::aleatory_uncertain_counts(), Variables::cv(), SharedVariablesData::design_counts(), Variables::div(), Variables::dsv(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), SharedVariablesData::state_counts(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().

size_t ccv_index_map (size_t ccv_index, const Variables & vars) [private]

offset active complement ccv_index to create index into all continuous arrays
maps index within complement of active continuous variables to index within all continuous variables.

References Dakota::abort_handler(), SharedVariablesData::aleatory_uncertain_counts(), SharedVariablesData::design_counts(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().

size_t cdiv_index_map (size_t cdiv_index, const Variables & vars) [private]

offset active complement cdiv_index to create index into all discrete int arrays
maps index within complement of active discrete int variables to index within all discrete int variables.

References Dakota::abort_handler(), SharedVariablesData::aleatory_uncertain_counts(), SharedVariablesData::design_counts(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().

size_t cdsv_index_map (size_t cdsv_index, const Variables & vars) [private]

offset active complement cdsv_index to create index into all discrete string arrays
maps index within complement of active discrete string variables to index within all discrete string variables.

References Dakota::abort_handler(), SharedVariablesData::aleatory_uncertain_counts(), SharedVariablesData::design_counts(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().

size_t cdrv_index_map (size_t cdrv_index, const Variables & vars) [private]

offset active complement cdrv_index to create index into all discrete real arrays
maps index within complement of active discrete real variables to index within all discrete real variables.

References Dakota::abort_handler(), SharedVariablesData::aleatory_uncertain_counts(), SharedVariablesData::design_counts(), SharedVariablesData::epistemic_uncertain_counts(), Variables::shared_data(), Dakota::svd(), and SharedVariablesData::view().

Referenced by NestedModel::NestedModel(), and NestedModel::update_sub_model().

void response_mapping (const Response & opt_interface_response, const Response & sub_iterator_response, Response & mapped_response) [inline], [private]

combine the response from the optional interface evaluation with the response from the sub-iteration using the primaryCoeffs/secondaryCoeffs mappings to create the total response for the model
In the OUU case,

optionalInterface fns = \{f\}, \{g\} (deterministic primary functions, constraints)
subIterator fns = \{S\} (UQ response statistics)

Problem formulation for mapped functions:
\[
\begin{align*}
\text{minimize} & \quad \{f\} + [W]\{S\} \\
\text{subject to} & \quad \{g\_l\} \leq \{g\} \leq \{g\_u\} \\
& \quad \{a\_l\} \leq [A]\{S\} \leq \{a\_u\} \\
& \quad \{g\} = \{g\_t\} \\
& \quad [A]\{S\} = \{a\_t\}
\end{align*}
\]

where [W] is the primary_mapping_matrix user input (primaryRespCoeffs class attribute), [A] is the secondary_mapping_matrix user input (secondaryRespCoeffs class attribute), \{\{g\_l\}, \{a\_l\}\} are the top level inequality constraint lower bounds, \{\{g\_u\}, \{a\_u\}\} are the top level inequality constraint upper bounds, and \{\{g\_t\}, \{a\_t\}\} are the top level equality constraint targets.

NOTE: optionalInterface/subIterator primary fns (obj/lsq/generic fns) overlap but optionalInterface/subIterator secondary fns (ineq/eq constraints) do not. The [W] matrix can be specified so as to allow

- some purely deterministic primary functions and some combined: [W] filled and [W].num_rows() < \{f\}.length() [combined first] or [W].num_rows() == \{f\}.length() and [W] contains rows of zeros [combined last]
- some combined and some purely stochastic primary functions: [W] filled and [W].num_rows() > \{f\}.length()
- separate deterministic and stochastic primary functions: [W].num_rows() > \{f\}.length() and [W] contains \{f\}.length() rows of zeros.

If the need arises, could change constraint definition to allow overlap as well: \{g\_l\} \leq \{g\} + [A]\{S\} \leq \{g\_u\}

with [A] usage the same as for [W] above.

In the UOO case, things are simpler, just compute statistics of each optimization response function: [W] = [I], \{f\}/[g]/[A] are empty.

References Response::active_set_request_vector(), NestedModel::check_response_map(), NestedModel::interface_response_overlay(), and NestedModel::iterator_response_overlay().

13.85.3 Member Data Documentation

Model subModel [private]

the sub-model used in sub-iterator evaluations

There are no restrictions on subModel, so arbitrary nestings are possible. This is commonly used to support surrogate-based optimization under uncertainty by having NestedModels contain SurrogateModels and vice versa.

Referred by NestedModel::component_parallel_mode(), NestedModel::derived_init_serial(), NestedModel::derived_subordinate_models(), NestedModel::estimate_partition_bounds(), NestedModel::fine_grained_evaluation_counters(), NestedModel::integer_variable_mapping(), NestedModel::NestedModel(), NestedModel::print_evaluation_summary(), NestedModel::real_variable_mapping(), NestedModel::resolve_integer_variable_mapping(), NestedModel::resolve_real_variable_mapping(), NestedModel::resolve_string_variable_mapping(), NestedModel::serve_run(), NestedModel::set_mapping(), NestedModel::sm_aciv_index_map(), NestedModel::sm_adiv_index_map(), NestedModel::sm_subordinate_model(), NestedModel::surrogate_response_mode(), NestedModel::update_inactive_view(), NestedModel::update_sub_model(), and NestedModel::warm_start_flag().

The documentation for this class was generated from the following files:

- NestedModel.hpp
- NestedModel.cpp
13.86  NIDRProblemDescDB Class Reference

The derived input file database utilizing the new IDR parser.

Inheritance diagram for NIDRProblemDescDB:

```
ProblemDescDB
\|-- NIDRProblemDescDB
```

Public Member Functions

- **NIDRProblemDescDB** (ParallelLibrary &parallel_lib)
  
  *constructor*

- **~NIDRProblemDescDB** ()
  
  *destructor*

- **void derived_parse_inputs** (const ProgramOptions &prog_opts)
  
  *parses the input file and populates the problem description database using NIDR.*

- **void derived_broadcast** ()
  
  *perform any data processing that must be coordinated with DB buffer broadcasting (performed prior to broadcast-
  ing the DB buffer on rank 0 and after receiving the DB buffer on other processor ranks)*

- **void derived_post_process** ()
  
  *perform any additional data post-processing*

- **KWH** (iface_Real)
- **KWH** (iface_Rlit)
- **KWH** (iface_false)
- **KWH** (iface_ilit)
- **KWH** (iface_pint)
- **KWH** (iface_lit)
- **KWH** (iface_start)
- **KWH** (iface_stop)
- **KWH** (iface_str)
- **KWH** (iface_str2D)
- **KWH** (iface_strL)
- **KWH** (iface_true)
- **KWH** (iface_type)
- **KWH** (method_Li)
- **KWH** (method_Real)
- **KWH** (method_Real01)
- **KWH** (method_RealDL)
- **KWH** (method_RealLlit)
- **KWH** (method_Realp)
- **KWH** (method_Realz)
- **KWH** (method_Ri)
- **KWH** (method_false)
CHAPTER 13. CLASS DOCUMENTATION

- **KWH** (method_szarray)
- **KWH** (method_ilit2)
- **KWH** (method_ilit2p)
- **KWH** (method_int)
- **KWH** (method_ivec)
- **KWH** (method_lit)
- **KWH** (method_litc)
- **KWH** (method_litp)
- **KWH** (method_lit)
- **KWH** (method_lit)
- **KWH** (method_order)
- **KWH** (method_num)
- **KWH** (method_num_resplevs)
- **KWH** (method_piecewise)
- **KWH** (method_pint)
- **KWH** (method_pintz)
- **KWH** (method_resplevs)
- **KWH** (method_resplevs01)
- **KWH** (method_shint)
- **KWH** (method_sizet)
- **KWH** (method_split2)
- **KWH** (method_start)
- **KWH** (method_stop)
- **KWH** (method_str)
- **KWH** (method_strL)
- **KWH** (method_true)
- **KWH** (method_tr_final)
- **KWH** (method_type)
- **KWH** (method_usharray)
- **KWH** (method_ushint)
- **KWH** (method_utype)
- **KWH** (method_augment_utype)
- **KWH** (method_utype_lit)
- **KWH** (model<Real>)
- **KWH** (model<RealDL>)
- **KWH** (model_ivec)
- **KWH** (model_false)
- **KWH** (model_int)
- **KWH** (model_intsetm1)
- **KWH** (model_lit)
- **KWH** (model_order)
- **KWH** (model_pint)
- **KWH** (model_pint)
- **KWH** (model_shint)
- **KWH** (model_start)
- **KWH** (model_stop)
• `KWH (model_str)`
• `KWH (model_strL)`
• `KWH (model_true)`
• `KWH (model_type)`
• `KWH (model_utype)`
• `KWH (model_augment_utype)`
• `KWH (resp_RealDL)`
• `KWH (resp_RealL)`
• `KWH (resp_false)`
• `KWH (resp_intset)`
• `KWH (resp_ivec)`
• `KWH (resp_lit)`
• `KWH (resp_sizet)`
• `KWH (resp_start)`
• `KWH (resp_stop)`
• `KWH (resp_str)`
• `KWH (resp_strL)`
• `KWH (resp_true)`
• `KWH (resp_utype)`
• `KWH (resp_augment_utype)`
• `KWH (env_int)`
• `KWH (env_start)`
• `KWH (env_str)`
• `KWH (env_strL)`
• `KWH (env_true)`
• `KWH (env_utype)`
• `KWH (env_augment_utype)`
• `KWH (var_RealLb)`
• `KWH (var_RealUb)`
• `KWH (var_IntLb)`
• `KWH (var_categorical)`
• `KWH (var_cauilbl)`
• `KWH (var_dauilbl)`
• `KWH (var_dauslbl)`
• `KWH (var_daurlbl)`
• `KWH (var_ceuilbl)`
• `KWH (var_deuilbl)`
• `KWH (var_deuslbl)`
• `KWH (var_deurlbl)`
• `KWH (var_pintz)`
• `KWH (var_start)`
• `KWH (var_stop)`
• `KWH (var_str)`
• `KWH (var_strL)`
• `KWH (var_true)`
• `KWH (var_newiarray)`
• KWH (var_newarray)
• KWH (var_newivec)
• KWH (var_newrvec)
• KWH (var_ivec)
• KWH (var_svec)
• KWH (var_rvec)
• KWH (var_type)

Static Public Member Functions

• static void botch (const char *fmt,...)
  print and error message and immediately abort
• static void check_variables (std::list<DataVariables> *)
  check each node in a list of DataVariables, first mapping DataVariables members back to flat NIDR arrays if needed.
• static void check_responses (std::list<DataResponses> *)
• static void check_descriptors (const StringArray &labels)
  Validate user-supplied descriptors.
• static void make_variable_defaults (std::list<DataVariables> *)
  Bounds and initial point check and inferred bounds generation.
• static void make_response_defaults (std::list<DataResponses> *)
• static void squawk (const char *fmt,...)
  print an error message and increment nerr, but continue
• static void warn (const char *fmt,...)
  print a warning

Static Public Attributes

• static NIDRProblemDescDB *pDDBInstance
  Pointer to the active object instance used within the static kwhandler functions in order to avoid the need for static data. Only initialized when parsing an input file; will be NULL for cases of direct DB population only.
• static int nerr = 0
  number of parse error encountered

Static Private Member Functions

• static void check_variables_node (void *)
  check a single variables node; input argument v is VarInfo
• static int check_driver (const String &an_driver, const StringArray &link_files, const StringArray &copy_files)
  tokenize and try to validate the presence of an analysis driver, potentially included in the linked or copied template files

Private Attributes

• std::list<void *> VIL
  List of VarInfo pointers, one per Variables instance.
Additional Inherited Members

13.86.1 Detailed Description

The derived input file database utilizing the new IDR parser.

The NIDRProblemDescDB class is derived from ProblemDescDB for use by the NIDR parser in processing DAKOTA input file data. For information on modifying the NIDR input parsing procedures, refer to Dakota/docs/Dev_Spec_Change.dox. For more on the parsing technology, see ”Specifying and Reading Program Input with NIDR” by David M. Gay (report SAND2008-2261P, which is available in PDF form as http://dakota.sandia.gov/papers/nidr08.pdf). Source for the routines declared herein is NIDRProblemDescDB.cpp, in which most routines are so short that a description seems unnecessary.

13.86.2 Member Function Documentation

void derived_parse_inputs ( const ProgramOptions & prog_opts ) [virtual]

parses the input file and populates the problem description database using NIDR.

Parse the input file using the Input Deck Reader (IDR) parsing system. IDR populates the IDRProblemDescDB object with the input file data.

Reimplemented from ProblemDescDB.

References Dakota::abort_handler(), NIDRProblemDescDB::botch(), ProblemDescDB::dataMethodList, DataMethodRep::dlDetails, DataMethodRep::dlLib, ProgramOptions::input_file(), ProgramOptions::input_string(), NIDRProblemDescDB::nerr, ProblemDescDB::parallel_library(), ProgramOptions::parser_options(), NIDRProblemDescDB::pDDBInstance, and NIDRProblemDescDB::squawk().

int check_driver ( const String & an_driver, const StringArray & link_files, const StringArray & copy_files ) [static], [private]

tokenize and try to validate the presence of an analysis driver, potentially included in the linked or copied template files

returns 1 if not found, 2 if found, but not executable, 0 if found (no error) in case we want to return to error on not found...

References WorkdirHelper::find_driver(), NIDRProblemDescDB::squawk(), WorkdirHelper::tokenize_driver(), NIDRProblemDescDB::warn(), and WorkdirHelper::which().

void make_variable_defaults ( std::list< DataVariables > * dvl ) [static]

Bounds and initial point check and inferred bounds generation.

Size arrays for contiguous storage of aggregated uncertain types. For each variable type, call Vgen_* to generate inferred bounds and initial point, repairing initial if needed. size the aggregate arrays for uncertain (design and state are stored separately

References Dakota::DesignAndStateLabelsCheck, NIDRProblemDescDB::squawk(), Dakota::var_mp_drange, Dakota::VLUncertainInt, Dakota::VLUncertainReal, and Dakota::VLUncertainStr.

Referenced by NIDRProblemDescDB::derived_post_process().

The documentation for this class was generated from the following files:

- NIDRProblemDescDB.hpp
- NIDRProblemDescDB.cpp
13.87 NL2Res Struct Reference

Auxiliary information passed to calcr and calcj via ur.

Public Attributes

- Real * r
  residual \( r = r(x) \)
- Real * J
  Jacobian \( J = J(x) \)
- Real * x
  corresponding parameter vector
- int nf
  function invocation count for \( r(x) \)

13.87.1 Detailed Description

Auxiliary information passed to calcr and calcj via ur.

The documentation for this struct was generated from the following file:
- NL2SOLLeastSq.cpp

13.88 NL2SOLLeastSq Class Reference

Wrapper class for the NL2SOL nonlinear least squares library.

Inheritance diagram for NL2SOLLeastSq:

```
  Itera
  
  Minimizer
  
  LeastSq
  
  NL2SOLLeastSq
```

Public Member Functions

- NL2SOLLeastSq (ProblemDescDB &problem_db, Model &model)
  standard constructor
- NL2SOLLeastSq (Model &model)
  alternate constructor
- ~NL2SOLLeastSq ()
  destructor
- void core_run ()
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Static Private Member Functions

- static void calc_r (int *np, int *pp, Real *x, int *nfp, Real *r, int *ui, void *ur, Vf vf)
  evaluator function for residual vector
- static void calc_j (int *np, int *pp, Real *x, int *nfp, Real *J, int *ui, void *ur, Vf vf)
  evaluator function for residual Jacobian

Private Attributes

- int auxprt
  auxiliary printing bits (see Dakota Ref Manual): sum of
  < 1 = x0prt (print initial guess) < 2 = solprt (print final solution) < 4 = statpr (print solution statistics) < 8 =
  parprt (print nondefault parameters) < 16 = dradpr (print bound constraint drops/adds) < debug/verbose/normal
  use default = 31 (everything), < quiet uses 3, silent uses 0.

- int outlev
  frequency of output summary lines in number of iterations
  < (debug/verbose/normal/quiet use default = 1, silent uses 0)

- Real dltfdj
  finite-diff step size for computing Jacobian approximation
  < (fd.gradient_step_size)

- Real delta0
  finite-diff step size for gradient differences for H
  < (a component of some covariance approximations, if desired) < (fd.hessian_step_size)

- Real dltfdc
  finite-diff step size for function differences for H
  < (fd.hessian_step_size)

- int mxfcal
  function-evaluation limit (max.function_evaluations)

- int mxiter
  iteration limit (max.iterations)

- Real rfctol
  relative fn convergence tolerance (convergence.tolerance)

- Real afctol
  absolute fn convergence tolerance (absolute_conv_tol)

- Real xctol
  x-convergence tolerance (x_conv_tol)

- Real sctol
  singular convergence tolerance (singular_conv_tol)

- Real lmaxs
  radius for singular-convergence test (singular.radius)

- Real xftol
  false-convergence tolerance (false_conv_tol)

- int covreq
  kind of covariance required (\c covariance):
  < 1 or -1 ==> sigma^2 2 H^{-1} J^T J H^{-1} < 2 or -2 ===> sigma^2 2 H^{-1} < 3 or -3 ===> sigma^2 2 (J^T J)^{-1}
  < 1 or 2 ===> use gradient diffs to estimate H < -1 or -2 ===> use function diffs to estimate H < default = 0 (no covariance)
• int rdreq
  whether to compute the regression diagnostic vector <(regression_diagnostics)
• Real fprec
  expected response function precision (function_precision)
• Real lmax0
  initial trust-region radius (initial_trust_radius)

Static Private Attributes
• static NL2SOLLeastSq * nl2solInstance
  pointer to the active object instance used within the static evaluator functions

Additional Inherited Members

13.88.1 Detailed Description
Wrapper class for the NL2SOL nonlinear least squares library.

The NL2SOLLeastSq class provides a wrapper for NL2SOL (TOMS Algorithm 573), in the updated form of Port Library routines dn[bfg] from Bell Labs; see http://www.netlib.org/port/readme. The Fortran from Port has been turned into C by f2c. NL2SOL uses a function pointer approach for which passed functions must be either global functions or static member functions.

13.88.2 Member Function Documentation

void core_run ( ) [virtual]
core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post


Reimplemented from Iterator.

References NL2SOLLeastSq::aftol, NL2SOLLeastSq::auxprt, Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::boundConstraintFlag, NL2SOLLeastSq::calcj(), NL2SOLLeastSq::calcr(), Minimizer::calibrationDataFlag, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Dakota::copy_data(), NL2SOLLeastSq::covreq, NL2SOLLeastSq::delta0, NL2SOLLeastSq::dltfdj, Minimizer::expData, NL2SOLLeastSq::fprec, Model::gradient_type(), ExperimentData::interpolate_flag(), Iterator::iteratedModel, NL2SOLLeastSq::lmax0, NL2SOLLeastSq::lmaxs, NL2SOLLeastSq::mxiter, NL2SOLLeastSq::mxcal, NL2SOLLeastSq::mxfer, NL2SOLLeastSq::nl2solInstance, Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, Minimizer::numUserPrimaryFns, NL2SOLLeastSq::outlev, NL2SOLLeastSq::rdreq, NL2SOLLeastSq::rfctol, NL2SOLLeastSq::scotol, Minimizer::speculativeFlag, Minimizer::vendorNumericalGradFlag, NL2SOLLeastSq::xctol, and NL2SOLLeastSq::xftol.

The documentation for this class was generated from the following files:

• NL2SOLLeastSq.hpp
• NL2SOLLeastSq.cpp
13.89 NLPQLPOptimizer Class Reference

Wrapper class for the NLPQLP optimization library, Version 2.0.

Inheritance diagram for NLPQLPOptimizer:

```
    NLPQLPOptimizer
     |                  |
     |                  |
     v                  v
Minimizer            Optimizer
     |                  |
     |                  |
     v                  v
Iterator
```

Public Member Functions

- `NLPQLPOptimizer (ProblemDescDB &problem_db, Model &model)`
  standard constructor
- `NLPQLPOptimizer (Model &model)`
  alternate constructor
- `~NLPQLPOptimizer ()`
  destructor
- `void core_run ()`
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Protected Member Functions

- `void initialize_run ()`
  performs run-time set up

Private Member Functions

- `void initialize ()`
  Shared constructor code.
- `void allocate_workspace ()`
  Allocates workspace for the optimizer.
- `void deallocate_workspace ()`
  Releases workspace memory.
- `void allocate_constraints ()`
  Allocates constraint mappings.
Private Attributes

- **int L**
  
  \( L \) : Number of parallel systems, i.e. function calls during line search at predetermined iterates. HINT: If only less than 10 parallel function evaluations are possible, it is recommended to apply the serial version by setting \( L=1 \).

- **int numEqConstraints**
  
  numEqConstraints : Number of equality constraints.

- **int MMAX**
  
  MMAX : Row dimension of array \( DG \) containing Jacobian of constraints. MMAX must be at least one and greater or equal to \( M \).

- **int N**
  
  N : Number of optimization variables.

- **int NMAX**
  
  NMAX : Row dimension of \( C \). NMAX must be at least two and greater than \( N \).

- **int MNN2**
  
  MNN2 : Must be equal to \( M+N+N+2 \).

- **double * X**
  
  \( X(NMAX,L) \) : Initially, the first column of \( X \) has to contain starting values for the optimal solution. On return, \( X \) is replaced by the current iterate. In the driving program the row dimension of \( X \) has to be equal to \( NMAX \). \( X \) is used internally to store \( L \) different arguments for which function values should be computed simultaneously.

- **double * F**
  
  \( F(L) \) : On return, \( F(1) \) contains the final objective function value. \( F \) is used also to store \( L \) different objective function values to be computed from \( L \) iterates stored in \( X \).

- **double * G**
  
  \( G(MMAX,L) \) : On return, the first column of \( G \) contains the constraint function values at the final iterate \( X \). In the driving program the row dimension of \( G \) has to be equal to \( MMAX \). \( G \) is used internally to store \( L \) different set of constraint function values to be computed from \( L \) iterates stored in \( X \).

- **double * DF**
  
  \( DF(NMAX) \) : \( DF \) contains the current gradient of the objective function. In case of numerical differentiation and a distributed system \( (L>1) \), it is recommended to apply parallel evaluations of \( F \) to compute \( DF \).

- **double * DG**
  
  \( DG(MMAX,NMAX) \) : \( DG \) contains the gradients of the active constraints \( (ACTIVE(J)=.true.) \) at a current iterate \( X \). The remaining rows are filled with previously computed gradients. In the driving program the row dimension of \( DG \) has to be equal to \( MMAX \).

- **double * U**
  
  \( U(MNN2) \) : \( U \) contains the multipliers with respect to the actual iterate stored in the first column of \( X \). The first \( M \) locations contain the multipliers of the \( M \) nonlinear constraints, the subsequent \( N \) locations the multipliers of the lower bounds, and the final \( N \) locations the multipliers of the upper bounds. At an optimal solution, all multipliers with respect to inequality constraints should be nonnegative.

- **double * C**
  
  \( C(NMAX,NMAX) \) : On return, \( C \) contains the last computed approximation of the Hessian matrix of the Lagrangian function stored in form of an LDL decomposition. \( C \) contains the lower triangular factor of an LDL factorization of the final quasi-Newton matrix (without diagonal elements, which are always one). In the driving program, the row dimension of \( C \) has to be equal to \( NMAX \).

- **double * D**
  
  \( D(NMAX) \) : The elements of the diagonal matrix of the LDL decomposition of the quasi-Newton matrix are stored in the one-dimensional array \( D \).
• double ACC

ACC : The user has to specify the desired final accuracy (e.g. 1.0D-7). The termination accuracy should not be smaller than the accuracy by which gradients are computed.

• double ACCQP

ACCQP : The tolerance is needed for the QP solver to perform several tests, for example whether optimality conditions are satisfied or whether a number is considered as zero or not. If ACCQP is less or equal to zero, then the machine precision is computed by NLPQLP and subsequently multiplied by 1.0D+4.

• double STPMIN

STPMIN : Minimum steplength in case of L>1. Recommended is any value in the order of the accuracy by which functions are computed. The value is needed to compute a steplength reduction factor by STPMIN**(1/L-1). If STPMIN<0, then STPMIN=ACC is used.

• int MAXFUN

MAXFUN : The integer variable defines an upper bound for the number of function calls during the line search (e.g. 20). MAXFUN is only needed in case of L=1, and must not be greater than 50.

• int MAXIT

MAXIT : Maximum number of outer iterations, where one iteration corresponds to one formulation and solution of the quadratic programming subproblem, or, alternatively, one evaluation of gradients (e.g. 100).

• int MAX_NM

MAX_NM : Stack size for storing merit function values at previous iterations for non-monotone line search (e.g. 10). In case of MAX_NM<0, monotone line search is performed.

• double TOL_NM

TOL_NM : Relative bound for increase of merit function value, if line search is not successful during the very first step. Must be non-negative (e.g. 0.1).

• int IPRINT

IPRINT : Specification of the desired output level. IPRINT = 0 : No output of the program. IPRINT = 1 : Only a final convergence analysis is given. IPRINT = 2 : One line of intermediate results is printed in each iteration. IPRINT = 3 : More detailed information is printed in each iteration step, e.g. variable, constraint and multiplier values. IPRINT = 4 : In addition to 'IPRINT=3', merit function and steplength values are displayed during the line search.

• int MODE

MODE : The parameter specifies the desired version of NLPQLP. MODE = 0 : Normal execution (reverse communication!). MODE = 1 : The user wants to provide an initial guess for the multipliers in U and for the Hessian of the Lagrangian function in C and D in form of an LDL decomposition.

• int IOUT

IOUT : Integer indicating the desired output unit number, i.e. all write-statements start with 'WRITE(IOUT,... '.

• int IFAIL

IFAIL : The parameter shows the reason for terminating a solution process. Initially IFAIL must be set to zero. On return IFAIL could contain the following values: IFAIL = -2 : Compute gradient values w.r.t. the variables stored in first column of X, and store them in DF and DG. Only derivatives for active constraints ACTIVE(J)=TRUE need to be computed. Then call NLPQLP again, see below. IFAIL = -1 : Compute objective fn and all constraint values subject the variables found in the first L columns of X, and store them in F and G. Then call NLPQLP again, see below. IFAIL = 0 : The optimality conditions are satisfied. IFAIL = 1 : The algorithm has been stopped after MAXIT iterations. IFAIL = 2 : The algorithm computed an uphill search direction. IFAIL = 3 : Underflow occurred when determining a new approximation matrix for the Hessian of the Lagrangian. IFAIL = 4 : The line search could not be terminated successfully. IFAIL = 5 : Length of a working array is too short. More detailed error information is obtained with 'IPRINT>0'. IFAIL = 6 : There are false dimensions, for example M>MMAX, N>NMAX, or MNN2>M+N+N+2. IFAIL = 7 : The search direction is close to zero, but the current iterate is still infeasible. IFAIL = 8 : The starting point violates a lower or upper bound. IFAIL = 9 : Wrong
input parameter, i.e., MODE, LDL decomposition in D and C (in case of MODE=1), IPRINT, IOUT IFAIL = 10:
Internal inconsistency of the quadratic subproblem, division by zero. IFAIL > 100: The solution of the quadratic
programming subproblem has been terminated with an error message and IFAIL is set to IFQL+100, where IFQL
denotes the index of an inconsistent constraint.

- double * WA
  WA(LWA) : WA is a real working array of length LWA.
- int LWA
  LWA : LWA value extracted from NLPQLP20.f.
- int * KWA
  KWA(LKWA) : The user has to provide working space for an integer array.
- int LKWA
  LKWA : LKWA should be at least N+10.
- int * ACTIVE
  ACTIVE(LACTIV) : The logical array shows a user the constraints, which NLPQLP considers to be active at the
  last computed iterate, i.e. G(J,X) is active, if and only if ACTIVE(J)=.TRUE., J=1,...,M.
- int LACTIVE
  LACTIV : The length LACTIV of the logical array should be at least 2+M+10.
- int LQL
  LQL : If LQL = .TRUE., the quadratic programming subproblem is to be solved with a full positive definite quasi-
  Newton matrix. Otherwise, a Cholesky decomposition is performed and updated, so that the subproblem matrix
  contains only an upper triangular factor.
- int numNlpqlConstr
  total number of constraints seen by NLPQL
- SizetList nonlinIneqConMappingIndices
  a list of indices for referencing the DAKOTA nonlinear inequality constraints used in computing the corresponding
  NLPQL constraints.
- RealList nonlinIneqConMappingMultipliers
  a list of multipliers for mapping the DAKOTA nonlinear inequality constraints to the corresponding NLPQL con-
  straints.
- RealList nonlinIneqConMappingOffsets
  a list of offsets for mapping the DAKOTA nonlinear inequality constraints to the corresponding NLPQL constrai
- SizetList linIneqConMappingIndices
  a list of indices for referencing the DAKOTA linear inequality constraints used in computing the corresponding
  NLPQL constraints.
- RealList linIneqConMappingMultipliers
  a list of multipliers for mapping the DAKOTA linear inequality constraints to the corresponding NLPQL con-
  straints.
- RealList linIneqConMappingOffsets
  a list of offsets for mapping the DAKOTA linear inequality constraints to the corresponding NLPQL constraints.

Additional Inherited Members

13.89.1 Detailed Description
Wrapper class for the NLPQLP optimization library, Version 2.0.
This subroutine solves the general nonlinear programming problem

\[
\begin{align*}
\text{minimize} & \quad F(X) \\
\text{subject to} & \quad G(J,X) = 0, \quad J=1,\ldots,ME \\
& \quad G(J,X) \geq 0, \quad J=ME+1,\ldots,M \\
& \quad XL \leq X \leq XU
\end{align*}
\]

and is an extension of the code NLPQLD. NLPQLP is specifically tuned to run under distributed systems. A new input parameter \( L \) is introduced for the number of parallel computers, that is the number of function calls to be executed simultaneously. In case of \( L=1 \), NLPQLP is identical to NLPQLD. Otherwise the line search is modified to allow \( L \) parallel function calls in advance. Moreover the user has the opportunity to used distributed function calls for evaluating gradients.

The algorithm is a modification of the method of Wilson, Han, and Powell. In each iteration step, a linearly constrained quadratic programming problem is formulated by approximating the Lagrangian function quadratically and by linearizing the constraints. Subsequently, a one-dimensional line search is performed with respect to an augmented Lagrangian merit function to obtain a new iterate. Also the modified line search algorithm guarantees convergence under the same assumptions as before.

For the new version, a non-monotone line search is implemented which allows to increase the merit function in case of instabilities, for example caused by round-off errors, errors in gradient approximations, etc.

The subroutine contains the option to predetermine initial guesses for the multipliers or the Hessian of the Lagrangian function and is called by reverse communication.

### 13.89.2 Member Function Documentation

**void core_run ( )** *virtual*

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from `Iterator`.

References NLPQLPOptimizer::ACC, NLPQLPOptimizer::ACCQP, NLPQLPOptimizer::ACTIVE, Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, NLPQLPOptimizer::C, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Dakota::copy_data(), Model::current_response(), NLPQLPOptimizer::D, NLPQLPOptimizer::deallocate_workspace(), NLPQLPOptimizer::DF, NLPQLPOptimizer::DG, Model::evaluate(), NLPQLPOptimizer::F, Response::function_gradients(), Response::function_values(), NLPQLPOptimizer::G, NLPQLPOptimizer::IFAIL, NLPQLPOptimizer::IOUT, NLPQLPOptimizer::IPRINT, Iterator::iteratedModel, NLPQLPOptimizer::KWA, NLPQLPOptimizer::L, NLPQLPOptimizer::LAC-TIVE, Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), NLPQLPOptimizer::linIneqConMappingIndices, NLPQLPOptimizer::linIneqConMappingOffsets, NLPQLPOptimizer::LKWA, Optimizer::localObjectiveRecast, NLPQLPOptimizer::LQL, NLPQLPOptimizer::LWA, NLPQLPOptimizer::MAX_NM, NLPQLPOptimizer::M-AxFUN, Iterator::maxFunctionEvals, NLPQLPOptimizer::MAXIT, NLPQLPOptimizer::MMAX, NLPQLPOptimizer::MNN2, NLPQLPOptimizer::MODE, NLPQLPOptimizer::N, NLPQLPOptimizer::NMAX, Model::nonlinear_eq_constraint_targets(), NLPQLPOptimizer::nonlinIneqConMappingIndices, NLPQLPOptimizer::nonlinIneqConMappingMultipliers, NLPQLPOptimizer::nonlinIneqConMappingOffsets, Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Minimizer::numContinuousVars, NLPQLPOptimizer::numEqConstrs, Minimizer::numFunctions, NLPQLPOptimizer::numNlpqlConstr, Optimizer::numObjectiveFns, Model::primary_response_fn_sense(), ActiveSet::request_value(), ActiveSet::request_values(), NLPQLPOptimizer::STPMIN, NLPQLPOptimizer::TOL_NM, NLPQLPOptimizer::U, NLPQLPOptimizer::WA, and NLPQLPOptimizer::X.

The documentation for this class was generated from the following files:
13.90 NLSSOLLeastSq Class Reference

Wrapper class for the NLSSOL nonlinear least squares library.

Inheritance diagram for NLSSOLLeastSq:

```
  Iterator
   ↓
  Minimizer
   ↓
LeastSq  SOLBase
   ▼
NLSSOLLeastSq
```

### Public Member Functions

- **NLSSOLLeastSq (ProblemDescDB &problem_db, Model &model)**
  
  *standard constructor*

- **NLSSOLLeastSq (Model &model)**
  
  *alternate constructor*

- **~NLSSOLLeastSq ()**
  
  *destructor*

- **void core_run ()**
  
  *core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post*

### Static Private Member Functions

- **static void least_sq_eval (int &mode, int &m, int &n, int &nrowfj, double *x, double *f, double *gradf, int &nstate)**
  
  *Evaluator for NLSSOL: computes the values and first derivatives of the least squares terms (passed by function pointer to NLSSOL).*

### Static Private Attributes

- **static NLSSOLLeastSq * nlssolInstance**
  
  *pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data*
Additional Inherited Members

13.90.1 Detailed Description

Wrapper class for the NLSSOL nonlinear least squares library.

The NLSSOLLeastSq class provides a wrapper for NLSSOL, a Fortran 77 sequential quadratic programming library from Stanford University marketed by Stanford Business Associates. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any nonstatic attribute used within static member functions must be either local to that function or accessed through a static pointer.

The user input mappings are as follows: max function evaluations is implemented directly in NLSSOLLeastSq's evaluator functions since there is no NLSSOL parameter equivalent, and max iterations, convergence tolerance, output verbosity, verify level, function precision, and linesearch tolerance are mapped into NLSSOL's "Major Iteration Limit", "Optimality Tolerance", "Major Print Level" (verbose: Major Print Level = 20; quiet: Major Print Level = 10), "Verify Level", "Function Precision", and "Linesearch Tolerance" parameters, respectively, using NLSSOL's npoptn() subroutine (as wrapped by npoptn2() from the npoptn wrapper.f file). Refer to [Gill, P.E., Murray, W., Saunders, M.A., and Wright, M.H., 1986] for information on NLSSOL's optional input parameters and the npoptn() subroutine.

13.90.2 Constructor & Destructor Documentation

NLSSOLLeastSq ( ProblemDescDB & problem_db, Model & model )

standard constructor
This is the primary constructor. It accepts a Model reference.
References Minimizer::constraintTol, Iterator::convergenceTol, Model::fd_gradient_step_size(), ProblemDescDB::get_int(), ProblemDescDB::get_real(), Model::gradient_type(), Iterator::iteratedModel, Iterator::maxIterations, Iterator::outputLevel, Iterator::probDescDB, SOLBase::set_options(), Minimizer::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

NLSSOLLeastSq ( Model & model )

alternate constructor
This is an alternate constructor which accepts a Model but does not have a supporting method specification from the ProblemDescDB.
References Minimizer::constraintTol, Iterator::convergenceTol, Model::fd_gradient_step_size(), Model::gradient_type(), Iterator::iteratedModel, Iterator::maxIterations, Iterator::outputLevel, SOLBase::set_options(), Minimizer::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

13.90.3 Member Function Documentation

void core_run ( ) [virtual]
core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
Reimplemented from Iterator.
References SOLBase::allocate_arrays(), SOLBase::allocate_workspace(), SOLBase::augment_bounds(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, SOLBase::cLambda, SOLBase::constraint_eval(), SOLBase::constraintJacMatrixF77, SOLBase::constraintState, SOLBase::constrOffset, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Dakota::copy_data(), Dakota::copy_data_partial(), SOLBase::deallocate_arrays(), Minimizer::expData, SOLBase::fnEvalCntr,
SOLBase::informResult, ExperimentData::interpolate_flag(), SOLBase::intWorkSpace, SOLBase::intWorkSpaceSize, Iterator::iteratedModel, NLSSOLLeastSq::least_sq_eval(), SOLBase::linConstraintArraySize, SOLBase::linConstraintMatrixF77, Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_upper_bounds(), SOLBase::nlnConstraintArraySize, NLSSOLLeastSq::nlssolInstance, Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_coeffs(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), SOLBase::numberIterations, Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, Minimizer::numLinearConstraints, Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, SOLBase::optLsqInstance, Minimizer::prevMinInstance, SOLBase::realWorkSpace, SOLBase::realWorkSpaceSize, SOLBase::solInstance, and SOLBase::upperFactorHessianF77.

The documentation for this class was generated from the following files:

- NLSSOLLeastSq.hpp
- NLSSOLLeastSq.cpp

### 13.91 NoDBBaseConstructor Struct Reference

Dummy struct for overloading constructors used in on-the-fly instantiations without ProblemDescDB support.

#### Public Member Functions

- **NoDBBaseConstructor** (int=0)

  C++ structs can have constructors.

#### 13.91.1 Detailed Description

Dummy struct for overloading constructors used in on-the-fly instantiations without ProblemDescDB support. **NoDBBaseConstructor** is used to overload the constructor used for on-the-fly instantiations in which ProblemDescDB queries cannot be used. Putting this struct here avoids circular dependencies.

The documentation for this struct was generated from the following file:

- dakota_global_defs.hpp

### 13.92 NomadOptimizer Class Reference

Wrapper class for NOMAD Optimizer.

Inheritance diagram for NomadOptimizer:

```
modalOptimizer
    |
    |
    Minimizer
    |
    |
    Optimizer
    |
    |
    Iterator
```
13.92. NOMADOPTIMIZER CLASS REFERENCE

Classes

- class Evaluator
  NOMAD-based Evaluator class.

Public Member Functions

- NomadOptimizer (ProblemDescDB &problem_db, Model &model)
  Constructor.
- NomadOptimizer (Model &model)
  alternate constructor for Iterator instantiations without DB
- ~NomadOptimizer ()
  Destructor.
- void core_run ()
  Calls the NOMAD solver.

Private Member Functions

- void load_parameters (Model &model, NOMAD::Parameters &p)
  Convenience function for Parameter loading.

Private Attributes

- int numTotalVars
  Total across all types of variables.
- int numNomadNonlinearIneqConstraints
  Number of nonlinear inequality constraints after put into the format required by NOMAD.
- int randomSeed
  Algorithm control parameters passed to NOMAD.
- int maxBlackBoxEvals
- int maxIterations
- Real initMesh
- Real minMesh
- Real epsilon
- Real vns
- std::string outputFormat
  Output control parameters passed to NOMAD.
- std::string historyFile
- bool displayAll
- int numHops
  Parameters needed for categorical neighbor construction.
- BitArray discreteSetIntCat
- BitArray discreteSetRealCat
- RealMatrixArray discreteSetIntAdj
- RealMatrixArray discreteSetRealAdj
- RealMatrixArray discreteSetStrAdj
CHAPTER 13. CLASS DOCUMENTATION

- RealMatrixArray `categoricalAdjacency`
- NOMAD::Point `initialPoint`
  Pointer to Nomad initial point.
- NOMAD::Point `upperBound`
  Pointer to Nomad upper bounds.
- NOMAD::Point `lowerBound`
  Pointer to Nomad lower bounds.
- `std::vector<int>` `constraintMapIndices`
  map from Dakota constraint number to Nomad constraint number
- `std::vector<double>` `constraintMapMultipliers`
  multipliers for constraint transformations
- `std::vector<double>` `constraintMapOffsets`
  offsets for constraint transformations
- `std::string` `useSurrogate`
  defines use of surrogate in NOMAD

Additional Inherited Members

13.92.1 Detailed Description

Wrapper class for NOMAD Optimizer.

NOMAD (is a Nonlinear Optimization by Mesh Adaptive Direct search) is a simulation-based optimization package designed to efficiently explore a design space using Mesh Adaptive Search.

Mesh Adaptive Direct Search uses Meshes, discretizations of the domain space of variables. It generates multiple meshes, and as its name implies, it also adapts the refinement of the meshes in order to find the best solution of a problem.

The objective of each iteration is to find points in a mesh that improves the current solution. If a better solution is not found, the next iteration is done over a finer mesh.

Each iteration is composed of two steps: Search and Poll. The Search step finds any point in the mesh in an attempt to find an improvement; while the Poll step generates trial mesh points surrounding the current best current solution.

The NomadOptimizer is a wrapper for the NOMAD library. It features the following attributes: `max_function_evaluations`, `display_format`, `display_all_evaluations`, `function_precision`, `max_iterations`.

13.92.2 Constructor & Destructor Documentation

`NomadOptimizer ( ProblemDescDB & problem_db, Model & model )`

Constructor.

- NOMAD Optimizer Constructor

  Parameters

  | model | DAKOTA Model object |

  References ProblemDescDB::get_ba(), ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_real(), ProblemDescDB::get_rma(), ProblemDescDB::get_string(), NomadOptimizer::numHops, NomadOptimizer::outputFormat, Iterator::probDescDB, NomadOptimizer::randomSeed, and NomadOptimizer::useSurrogate.
13.92.3 Member Function Documentation

```cpp
void load_parameters ( Model & model, NOMAD::Parameters & p ) [private]
```

Convenience function for Parameter loading.

This function takes the Parameters provided by the user in the DAKOTA model.

Parameters

| model | NOMAD Model object Variables for the stuff that must go in the parameters. Will be filled by calling load_parameters after the constructor to capture model recasts. |


Referenced by NomadOptimizer:::core_run().

The documentation for this class was generated from the following files:

- NomadOptimizer.hpp
- NomadOptimizer.cpp

13.93 NonD Class Reference

Base class for all nondeterministic iterators (the DAKOTA/UQ branch).

Inheritance diagram for NonD:
Public Member Functions

- void initialize_random_variables (short u_space_type)
  initialize natafTransform based on distribution data from iteratedModel
- void initialize_random_variables (const Pecos::ProbabilityTransformation &transform, bool deep_copy=false)
  alternate form: initialize natafTransform based on incoming data
- void initialize_random_variable_transformation ()
  instantiate natafTransform
- void initialize_random_variable_types ()
  initializes ranVarTypesX within natafTransform (u-space not needed)
- void initialize_random_variable_types (short u_space_type)
  initializes ranVarTypesX and ranVarTypesU within natafTransform
- void initialize_random_variable_parameters ()
  initializes ranVarMeansX, ranVarStdDevsX, ranVarLowerBndsX, ranVarUpperBndsX, and ranVarAddtlParamsX within natafTransform
- void initialize_random_variable_correlations ()
  propagate iteratedModel correlations to natafTransform
- void verify_correlation_support (short u_space_type)
  verify that correlation warping is supported by Nataf for given variable types
• void transform_correlations ()
  
  perform correlation warping for variable types supported by Nataf

• void requested_levels (const RealVectorArray &req_resp_levels, const RealVectorArray &req_prob_levels, const RealVectorArray &req_rel_levels, const RealVectorArray &req_gen_rel_levels, short resp_level_tgt, short resp_level_tgt_reduce, bool cdf_flag, bool pdf_output)
  
  set requestedRespLevels, requestedProbLevels, requestedRelLevels, requestedGenRelLevels, respLevelTarget, cdfFlag, and pdfOutput (used in combination with alternate ctors)

• void distribution_parameter_derivatives (bool dist_param_derivs)
  
  set distParamDerivs

• void print_level_mappings (std::ostream &s, String qoi_type, const StringArray &qoi_labels) const
  
  prints the z/p/beta/beta* mappings reflected in {requested,computed} {Resp,Prob,Rel,GenRel} Levels for default qoi_type and qoi_labels

• bool resize ()
  
  reinitializes iterator based on new variable size

• bool pdf_output () const
  
  get pdfOutput

• void pdf_output (bool output)
  
  set pdfOutput

• short final_moments_type () const
  
  get finalMomentsType

• void final_moments_type (short type)
  
  set finalMomentsType

• Pecos::ProbabilityTransformation & variable_transformation ()
  
  return natafTransform

**Protected Member Functions**

• NonD (ProblemDescDB &problem_db, Model &model)
  
  constructor

• NonD (unsigned short method_name, Model &model)
  
  alternate constructor for sample generation and evaluation "on the fly"

• NonD (unsigned short method_name, const RealVector &lower_bnds, const RealVector &upper_bnds)
  
  alternate constructor for sample generation "on the fly"

• ~NonD ()
  
  destructor

• void derived_set_communicators (ParLevLIter pl_iter)
  
  derived class contributions to setting the communicators associated with this Iterator instance

• void initialize_run ()
  
  utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

• void finalize_run ()
  
  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
• const Response & response_results () const
  return the final statistics from the nondeterministic iteration
• void response_results_active (const ActiveSet &set)
  set the active set within finalStatistics
• virtual void initialize_response_covariance ()
  initializes respCovariance
• virtual void initialize_final_statistics ()
  initializes finalStatistics for storing NonD final results
• virtual void update_final_statistics ()
  update finalStatistics::functionValues
• void size ()
  Size local variables.
• int generate_system_seed ()
  create a system-generated unique seed (when a seed is unspecified)
• void initialize_final_statistics_gradients ()
  initializes finalStatistics::functionGradients
• void update_aleatory_final_statistics ()
  update finalStatistics::functionValues from finalMomentStats and computed
  {Prob,Rel,GenRel,Resp} Levels
• void update_system_final_statistics ()
  update system metrics from component metrics within finalStatistics
• void update_system_final_statistics_gradients ()
  update finalStatistics::functionGradients
• void initialize_level_mappings ()
  size computed
  {Resp,Prob,Rel,GenRel} Levels
• void compute_densities (const RealRealPairArray &min_max_fns, bool prob_refinement=false, bool all_{levels,computed}=false)
  compute the PDF bins from the CDF/CCDF values and store in computedPDF
  {Abscissas,Ordinates}
• void print_densities (std::ostream &s) const
  output the PDFs reflected in computedPDF
  {Abscissas,Ordinates} using default qoi_type and pdf_label
• void print_densities (std::ostream &s, String qoi_type, const StringArray &pdf_labels) const
  output the PDFs reflected in computedPDF
  {Abscissas,Ordinates}
• void print_system_mappings (std::ostream &s) const
  print system series/parallel mappings for response levels
• void print_multilevel_evaluation_summary (std::ostream &s, const SizetArray &N_samp)
  print evaluation summary for multilevel sampling across 1D profile
• void print_multilevel_evaluation_summary (std::ostream &s, const Sizet2DArray &N_samp)
  print evaluation summary for multilevel sampling across 2D profile
• void print_multilevel_evaluation_summary (std::ostream &s, const Sizet3DArray &N_samp)
  print evaluation summary for multilevel sampling across 3D profile
• void transform_model (Model &x_model, Model &u_model, bool truncated_bounds=false, Real bound=10.)
  recast x_model from x-space to u-space to create u_model
• void construct_lhs (Iterator &u_space_sampler, Model &u_model, unsigned short sample_type, int num_{samples, int seed, const String &rng, bool vary_pattern, short sampling_{vars_mode}=ACTIVE)
assign a NonDLHSSampling instance within u_space_sampler

- void archive_allocate_mappings ()
  allocate results array storage for distribution mappings
- void archive_from_resp (size_t fn_index)
  archive the mappings from specified response levels for specified fn
- void archive_to_resp (size_t fn_index)
  allocate the mappings to computed response levels for specified fn
- void archive_allocate_pdf ()
  allocate results array storage for pdf histograms
- void archive_pdf (size_t fn_index)
  archive a single pdf histogram for specified function

Static Protected Member Functions

- static void vars_u_to_x_mapping (const Variables &u_vars, Variables &x_vars)
  static function for RecastModels used for forward mapping of u-space variables from NonD Iterators to x-space variables for Model evaluations
- static void vars_x_to_u_mapping (const Variables &x_vars, Variables &u_vars)
  static function for RecastModels used for inverse mapping of x-space variables from data import to u-space variables for NonD Iterators
- static void set_u_to_x_mapping (const Variables &u_vars, const ActiveSet &u_set, ActiveSet &x_set)
  static function for RecastModels used to map u-space ActiveSets from NonD Iterators to x-space ActiveSets for Model evaluations
- static void resp_x_to_u_mapping (const Variables &x_vars, const Variables &u_vars, const Response &x_response, Response &u_response)
  static function for RecastModels used to map x-space responses from Model evaluations to u-space responses for return to NonD Iterator.

Protected Attributes

- NonD * prevNondInstance
  pointer containing previous value of nondInstance
- Pecos::ProbabilityTransformation natafTransform
  Nonlinear variable transformation that encapsulates the required data for performing transformations from X -> Z -> U and back.
- size_t numContDesVars
  number of continuous design variables (modeled using uniform distribution for All view modes)
- size_t numDiscIntDesVars
  number of discrete integer design variables (modeled using discrete histogram distributions for All view modes)
- size_t numDiscStringDesVars
  number of discrete string design variables (modeled using discrete histogram distributions for All view modes)
- size_t numDiscRealDesVars
  number of discrete real design variables (modeled using discrete histogram distributions for All view modes)
- size_t numDesignVars
  total number of design variables
• `size_t numContStateVars`
  number of continuous state variables (modeled using uniform distribution for All view modes)

• `size_t numDiscIntStateVars`
  number of discrete integer state variables (modeled using discrete histogram distributions for All view modes)

• `size_t numDiscStringStateVars`
  number of discrete string state variables (modeled using discrete histogram distributions for All view modes)

• `size_t numDiscRealStateVars`
  number of discrete real state variables (modeled using discrete histogram distributions for All view modes)

• `size_t numStateVars`
  total number of state variables

• `size_t numNormalVars`
  number of normal uncertain variables (native space)

• `size_t numLognormalVars`
  number of lognormal uncertain variables (native space)

• `size_t numUniformVars`
  number of uniform uncertain variables (native space)

• `size_t numLoguniformVars`
  number of loguniform uncertain variables (native space)

• `size_t numTriangularVars`
  number of triangular uncertain variables (native space)

• `size_t numExponentialVars`
  number of exponential uncertain variables (native space)

• `size_t numBetaVars`
  number of beta uncertain variables (native space)

• `size_t numGammaVars`
  number of gamma uncertain variables (native space)

• `size_t numGumbelVars`
  number of gumbel uncertain variables (native space)

• `size_t numFrechetVars`
  number of frechet uncertain variables (native space)

• `size_t numWeibullVars`
  number of weibull uncertain variables (native space)

• `size_t numHistogramBinVars`
  number of histogram bin uncertain variables (native space)

• `size_t numPoissonVars`
  number of Poisson uncertain variables (native space)

• `size_t numBinomialVars`
  number of binomial uncertain variables (native space)

• `size_t numNegBinomialVars`
  number of negative binomial uncertain variables (native space)

• `size_t numGeometricVars`
  number of geometric uncertain variables (native space)

• `size_t numHyperGeomVars`
number of hypergeometric uncertain variables (native space)

- size_t numHistogramPtIntVars
  number of histogram point integer uncertain variables (native space)

- size_t numHistogramPtStringVars
  number of histogram point string uncertain variables (native space)

- size_t numHistogramPtRealVars
  number of histogram point real uncertain variables (native space)

- size_t numContIntervalVars
  number of continuous interval uncertain variables (native space)

- size_t numDiscIntervalVars
  number of discrete interval uncertain variables (native space)

- size_t numDiscSetIntUncVars
  number of discrete integer set uncertain variables (native space)

- size_t numDiscSetStringUncVars
  number of discrete integer set uncertain variables (native space)

- size_t numDiscSetRealUncVars
  number of discrete real set uncertain variables (native space)

- size_t numContAleatUncVars
  total number of continuous aleatory uncertain variables (native space)

- size_t numDiscIntAleatUncVars
  total number of discrete integer aleatory uncertain variables (native space)

- size_t numDiscStringAleatUncVars
  total number of discrete string aleatory uncertain variables (native space)

- size_t numDiscRealAleatUncVars
  total number of discrete real aleatory uncertain variables (native space)

- size_t numAleatoryUncVars
  total number of aleatory uncertain variables (native space)

- size_t numContEpistUncVars
  total number of continuous epistemic uncertain variables (native space)

- size_t numDiscIntEpistUncVars
  total number of discrete integer epistemic uncertain variables (native space)

- size_t numDiscStringEpistUncVars
  total number of discrete string epistemic uncertain variables (native space)

- size_t numDiscRealEpistUncVars
  total number of discrete real epistemic uncertain variables (native space)

- size_t numEpistemicUncVars
  total number of epistemic uncertain variables (native space)

- size_t numUncertainVars
  total number of uncertain variables (native space)

- bool epistemicStats
  flag for computing interval-type metrics instead of integrated metrics If any epistemic variables are active in a metric evaluation, then this flag is set.

- RealMatrix finalMomentStats
standardized or central moments of response functions, as determined by finalMomentsType. Calculated in compute-
moments() and indexed as (moment, fn).

- **RealVectorArray `requestedRespLevels`**
  requested response levels for all response functions

- **RealVectorArray `computedProbLevels`**
  output probability levels for all response functions resulting from `requestedRespLevels`

- **RealVectorArray `computedRelLevels`**
  output reliability levels for all response functions resulting from `requestedRespLevels`

- **RealVectorArray `computedGenRelLevels`**
  output generalized reliability levels for all response functions resulting from `requestedRespLevels`

- **short `respLevelTarget`**
  indicates mapping of $z \rightarrow p$ (PROBABILITIES), $z \rightarrow \beta$ (RELIABILITIES), or $z \rightarrow \beta^*$ (GEN_RELIABILITIES)

- **short `respLevelTargetReduce`**
  indicates component or system series/parallel failure metrics

- **RealVectorArray `requestedProbLevels`**
  requested probability levels for all response functions

- **RealVectorArray `requestedRelLevels`**
  requested reliability levels for all response functions

- **RealVectorArray `requestedGenRelLevels`**
  requested generalized reliability levels for all response functions

- **RealVectorArray `computedRespLevels`**
  output response levels for all response functions resulting from `requestedProbLevels`, `requestedRelLevels`, or `requestedGenRelLevels`

- **size_t `totalLevelRequests`**
  total number of levels specified within `requestedRespLevels`, `requestedProbLevels`, and `requestedRelLevels`

- **bool `cdfFlag`**
  flag for type of probabilities/reliabilities used in mappings: cumulative/CDF (true) or complementary/CCDF (false)

- **bool `pdfOutput`**
  flag for managing output of response probability density functions (PDFs)

- **RealVectorArray `computedPDFAbscissas`**
  sorted response PDF intervals bounds extracted from min/max sample and requested/computedRespLevels (vector lengths = num bins + 1)

- **RealVectorArray `computedPDFOrdinates`**
  response PDF densities computed from bin counts divided by (unequal) bin widths (vector lengths = num bins)

- **Response `finalStatistics`**
  final statistics from the uncertainty propagation used in strategies: response means, standard deviations, and probabilities of failure

- **short `finalMomentsType`**
  type of moments logged within `finalStatistics`: none, central, standard

- **size_t `miPLIndex`**
  index for the active `ParallelLevel` within `ParallelConfiguration::miPLIters`
Static Protected Attributes

- static NonD * nondInstance
  pointer to the active object instance used within static evaluator functions in order to avoid the need for static data

Private Member Functions

- void distribute_levels (RealVectorArray &levels, bool ascending=true)
  convenience function for distributing a vector of levels among multiple response functions if a short-hand specification is employed.
- void level_mappings_file (size_t fn_index, const String &qoi_label) const
  Write level mappings to a file for a single response.
- void print_level_map (std::ostream &s, size_t fn_index, const String &qoi_label) const
  Print level mapping for a single response function to ostream.
- unsigned short pecos_to_dakota_variable_type (unsigned short pecos_var_type)
  convert from Pecos To Dakota variable enumeration type for continuous aleatory uncertain variables used in variable transformations
- bool homogeneous (const SizetArray &N_l) const
  return true if N_l has consistent values

Private Attributes

- bool distParamDerivs
  flags calculation of derivatives with respect to distribution parameters s within resp_x_to_u_mapping() using the chain rule df/dx dx/ds. The default is to calculate derivatives with respect to standard random variables u using the chain rule df/dx dx/du.

13.93.1 Detailed Description

Base class for all nondeterministic iterators (the DAKOTA/UQ branch).

The base class for nondeterministic iterators consolidates uncertain variable data and probabilistic utilities for inherited classes.

13.93.2 Member Function Documentation

void initialize_random_variables ( short u_space_type )
initialize natafTransform based on distribution data from iteratedModel

Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.

References NonD::initialize_random_variable_correlations(), NonD::initialize_random_variable_parameters(), NonD::initialize_random_variable_transformation(), NonD::initialize_random_variable_types(), and NonD::verify_correlation_support().

Referenced by NonDExpansion::construct_expansion_sampler(), NonDBayesCalibration::construct_mcmc_model(), NonDExpansion::initialize_u_space_model(), NonDAdaptImpSampling::NonDAdaptImpSampling(), NonDGlobalReliability::NonDGlobalReliability(), NonDLocalReliability::NonDLocalReliability(), and NonDLHS-Sampling::pre_run().
void initialize_random_variables ( const Pecos::ProbabilityTransformation & transform, bool deep_copy = false )

alternate form: initialize natafTransform based on incoming data

This function is commonly used to publish transformation data when the Model variables are in a transformed space (e.g., u-space) and ProbabilityTransformation::ranVarTypes et al. may not be generated directly. This allows for the use of inverse transformations to return the transformed space variables to their original states.

References NonD::initialize_random_variable_transformation(), NonD::natafTransform, NonD::numContDesVars, NonD::numContEpistUncVars, NonD::numContIntervalVars, and NonD::numContStateVars.

void initialize_random_variable_types()

initializes ranVarTypesX within natafTransform (u-space not needed)

Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.

References Model::aleatory_distribution_parameters(), Model::cv(), Iterator::iteratedModel, NonD::natafTransform, NonD::numBetaVars, NonD::numBinomialVars, NonD::numContDesVars, NonD::numContIntervalVars, NonD::numContStateVars, NonD::numExponentialVars, NonD::numFrechetVars, NonD::numGammaVars, NonD::numGeometricVars, NonD::numGumbelVars, NonD::numHistogramBinVars, NonD::numHyperGeomVars, NonD::numLognormalVars, NonD::numLoguniformVars, NonD::numNegBinomialVars, NonD::numNormalVars, NonD::numPoissonVars, NonD::numTriangularVars, NonD::numUniformVars, and NonD::numWeibullVars.

Referenced by NonDExpansion::initialize(), NonD::initialize_random_variables(), NonDBayesCalibration::NonDBayesCalibration(), NonDIntegration::NonDIntegration(), NonDReliability::NonDReliability(), NonDLHSSampling::pre_run, and NonDReliability::resize().

void initialize_random_variable_types ( short u_space_type )

initializes ranVarTypesX and ranVarTypesU within natafTransform

Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.

References Dakota::abort_handler(), Model::aleatory_distribution_parameters(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), Iterator::iteratedModel, NonD::natafTransform, NonD::numBetaVars, NonD::numBinomialVars, NonD::numContDesVars, NonD::numContIntervalVars, NonD::numContStateVars, NonD::numExponentialVars, NonD::numFrechetVars, NonD::numGammaVars, NonD::numGeometricVars, NonD::numGumbelVars, NonD::numHistogramBinVars, NonD::numHyperGeomVars, NonD::numLognormalVars, NonD::numLoguniformVars, NonD::numNegBinomialVars, NonD::numNormalVars, NonD::numPoissonVars, NonD::numTriangularVars, NonD::numUniformVars, and NonD::numWeibullVars.

void initialize_random_variable_parameters()

initializes ranVarMeansX, ranVarStdDevsX, ranVarLowerBndsX, ranVarUpperBndsX, and ranVarAddtlParamsX within natafTransform

Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.

References Model::aleatory_distribution_parameters(), Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::epistemic_distribution_parameters(), Iterator::iteratedModel, NonD::natafTransform, NonD::numAleatoryUncVars, NonD::numContDesVars, Analyzer::numContinuousVars, NonD::numContStateVars, and NonD::numEpistemicUncVars.
Referenced by NonDGlobalReliability::core_run(), NonDExpansion::initialize_expansion(), NonDBayesCalibration-::initialize_model(), NonD::initialize_random_variables(), NonDLocalReliability::mean_value(), NonDLocalReliability-::mpp_search(), and NonDLHSSampling::pre_run.

```cpp
void print_level_mappings ( std::ostream & s, String qoi_type, const StringArray & qoi_labels ) const
```
prints the z/p/beta/beta∗ mappings reflected in \{requested,computed\}\{Resp,Prob,Rel,GenRel\} Levels
Print distribution mappings, including to file per response.
References NonD::level_mappings_file(), Analyzer::numFunctions, Iterator::outputLevel, NonD::print_densities(), NonD::print_level_map(), NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, and Dakota::write_precision.

```cpp
void initialize_run ( ) [inline], [protected], [virtual]
```
utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s initialize_run(), typically before performing its own implementation steps.
Reimplemented from Analyzer.
References Analyzer::initialize_run(), NonD::nondInstance, and NonD::prevNondInstance.

```cpp
void finalize_run ( ) [inline], [protected], [virtual]
```
utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s finalize_run(), typically after performing its own implementation steps.
Reimplemented from Analyzer.
References Analyzer::finalize_run(), NonD::nondInstance, and NonD::prevNondInstance.

```cpp
void initialize_final_statistics ( ) [protected], [virtual]
```
initializes finalStatistics for storing NonD final results
Default definition of virtual function (used by sampling, reliability, and stochastic expansion methods) defines the set of statistical results to include means, standard deviations, and level mappings.
Reimplemented in NonDIInterval.
References Dakota::abort_handler(), NonD::cdfFlag, Model::cv(), ActiveSet::derivative_vector(), NonD::epistemicStats, NonD::finalMomentsType, NonD::finalStatistics, Response::function_labels(), Model::inactive_continuous_variable_ids(), Iterator::iteratedModel, Analyzer::numFunctions, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, NonD::respLevelTargetReduce, and NonD::totalLevelRequests.
Referenced by NonDExpansion::NonDExpansion(), NonDIntegration::NonDIntegration(), NonDReliability-::NonDReliability(), NonDSampling::NonDSampling(), NonD::requested_levels(), and NonDReliability::resize().

```cpp
void compute_densities ( const RealRealPairArray & min_max_fns, bool prob_refinement = false, bool all_levels_computed = false ) [protected]
```
compute the PDF bins from the CDF/CCDF values and store in computedPDF\{Abscissas,Ordinates\}
This function infers PDFs from the CDF/CCDF level mappings, in order to enable PDF computation after CDF/CCDF probability level refinement (e.g., from importance sampling).
prob_refinement alerts the routine to exclude inverse mappings from the PDF, since refinement only applies to \( z \rightarrow p \) forward mappings and mixing refined and unrefined probability mappings results in an inconsistency (potentially manifesting as negative density values).

all_levels_computed is an option used by reliability methods where computed\( \ast \)_levels are defined across the union of all requested levels.

References NonD::archive_allocate_pdf(), NonD::archive_pdf(), NonD::cdfFlag, NonD::computedGenRelLevels, NonD::computedPDFAbscissas, NonD::computedPDFOrdinates, NonD::computedProbLevels, NonD::computedRespLevels, Analyzer::numFunctions, NonD::pdfOutput, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, and NonD::respLevelTarget.

Referenced by NonDSampling::compute_level_mappings(), NonDExpansion::compute_numerical_statistics(), NonDAdaptImpSampling::core_run(), NonDLocalReliability::core_run(), and NonDGlobalReliability::importance_sampling().

```cpp
void vars_u_to_x_mapping ( const Variables & u_vars, Variables & x_vars ) [inline], [static], [protected]
static function for RecastModels used for forward mapping of u-space variables from NonD Iterators to x-space variables for Model evaluations
  Map the variables from iterator space (u) to simulation space (x).
  References Variables::continuous_variables(), Variables::continuous_variables_view(), NonD::natafTransform, and NonD::nondInstance.
  Referenced by NonD::transform_model().
```

```cpp
void vars_x_to_u_mapping ( const Variables & x_vars, Variables & u_vars ) [inline], [static], [protected]
static function for RecastModels used for inverse mapping of x-space variables from data import to u-space variables for NonD Iterators
  Map the variables from simulation space (x) to iterator space (u).
  References Variables::continuous_variables(), Variables::continuous_variables_view(), NonD::natafTransform, and NonD::nondInstance.
  Referenced by NonD::transform_model().
```

```cpp
void set_u_to_x_mapping ( const Variables & u_vars, const ActiveSet & u_set, ActiveSet & x_set ) [static], [protected]
static function for RecastModels used to map u-space ActiveSets from NonD Iterators to x-space ActiveSets for Model evaluations
  Define the DVV for x-space derivative evaluations by augmenting the iterator requests to account for correlations.
  References Dakota::NPOS, Variables::all_continuous_variable_ids(), Dakota::contains(), Variables::continuous_variable_ids(), ActiveSet::derivative_vector(), Dakota::find_index(), Variables::inactive_continuous_variable_ids(), NonD::natafTransform, and NonD::nondInstance.
  Referenced by NonD::transform_model().
```

```cpp
void level_mappings_file ( size_t fn_index, const String & qoi_label ) const [private]
Write level mappings to a file for a single response.
  Write distribution mappings to a file for a single response.
  References NonD::print_level_map(), and Dakota::write_precision.
  Referenced by NonD::print_level_mappings().
```
void print_level_map ( std::ostream & s, size_t fn_index, const String & qoi_label ) const  [private]

Print level mapping for a single response function to ostream.

Print the distribution mapping for a single response function to the passed output stream. This base class version maps from one requested level type to one computed level type; some derived class implementations (e.g., local and global reliability) output multiple computed level types.

References NonD::cdfFlag, NonD::computedGenRelLevels, NonD::computedProbLevels, NonD::computed-RelLevels, NonD::computedRespLevels, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requested-RelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, and Dakota::write_precision.

Referenced by NonD::level_mappings_file(), and NonD::print_level_mappings().

The documentation for this class was generated from the following files:

- DakotaNonD.hpp
- DakotaNonD.cpp

13.94 NonDAdaptImpSampling Class Reference

Class for the Adaptive Importance Sampling methods within DAKOTA.

Inheritance diagram for NonDAdaptImpSampling:

```
Analyzer

NonD

NonDSampling

NonDAdaptImpSampling
```

Public Member Functions

- **NonDAdaptImpSampling (ProblemDescDB &problem_db, Model &model)**
  
  *standard constructor*

- **NonDAdaptImpSampling (Model &model, unsigned short sample_type, int samples, int seed, const String &rng, bool vary_pattern, unsigned short is_type, bool cdf_flag, bool x_space_model, bool use_model_bounds, bool track_extreme)**
  
  *alternate constructor for on-the-fly instantiations*

- **~NonDAdaptImpSampling ()**
  
  *destructor*

- **bool resize ()**
  
  *reinitializes iterator based on new variable size*

- **void derived_init_communicators (ParLevLIter pl_iter)**
  
  *derived class contributions to initializing the communicators associated with this Iterator instance*
• void derived_set_communicators (ParLevLIter pl_iter)
  derived class contributions to setting the communicators associated with this Iterator instance
• void derived_free_communicators (ParLevLIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance
• void core_run ()
  performs adaptive importance sampling and computes probability of failure
• void print_results (std::ostream &s)
  print the final statistics
• void initialize (const RealVectorArray &full_points, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)
  initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations
• void initialize (const RealMatrix &full_points, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)
  initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations
• void initialize (const RealVector &full_point, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)
  initializes data needed for importance sampling: an initial point around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations
• Real final_probability ()
  returns the final probability calculated by the importance sampling
• const RealRealPairArray & extreme_values () const
  return extremeValues

Private Member Functions

• void select_rep_points (const RealVectorArray &var_samples_u, const RealVector &fn_samples)
  select representative points from a set of samples
• void converge_statistics (bool cov_flag)
  iteratively generate samples and select representative points until probability and (optionally) coefficient of variation converge
• void generate_samples (RealVectorArray &var_samples_u)
  generate a set of samples based on multimodal sampling density
• void evaluate_samples (const RealVectorArray &var_samples_u, RealVector &fn_samples)
  evaluate the model at the sample points and store the responses
• void calculate_statistics (const RealVectorArray &var_samples_u, const RealVector &fn_samples, size_t total_samples, Real &sum_prob, Real &prob, bool compute_cov, Real &sum_var, Real &cov)
  calculate the probability of exceeding the failure threshold and the coefficient of variation (if requested)
• Real distance (const RealVector &a, const RealVector &b)
  compute Euclidean distance between points a and b
• Real recentered_density (const RealVector &sample_point)
  compute density between a representative point and a sample point, assuming standard normal
13.94. NONDADAPTIMPSAMPLING CLASS REFERENCE

Private Attributes

- **Model uSpaceModel**
  
  *importance sampling is performed in standardized probability space. This u-space model is either passed in (alternate constructor for helper AIS) or constructed using transform_model() (standard constructor for stand-alone AIS)*

- **unsigned short importanceSamplingType**
  
  *integration type (is, ais, mmais) provided by input specification*

- **bool initLHS**
  
  *flag to identify if initial points are generated from an LHS sample*

- **bool useModelBounds**
  
  *flag to control if the sampler should respect the model bounds*

- **bool invertProb**
  
  *flag for inversion of probability values using 1.-p*

- **bool trackExtremeValues**
  
  *flag for tracking min/max values encountered when evaluating samples*

- **int refineSamples**
  
  *size of sample batch within each refinement iteration*

- **size_t respFnIndex**
  
  *the active response function index in the model to be sampled*

- **RealVector designPoint**
  
  *design subset for which uncertain subset is being sampled*

- **RealVectorArray initPointsU**
  
  *the original set of u-space samples passed in initialize()*

- **RealVectorArray repPointsU**
  
  *the set of representative points in u-space around which to sample*

- **RealVector repWeights**
  
  *the weight associated with each representative point*

- **Real probEstimate**
  
  *the probability estimate that is iteratively refined by importance sampling*

- **Real failThresh**
  
  *the failure threshold (z-bar) for the problem.*

Additional Inherited Members

13.94.1 Detailed Description

Class for the Adaptive Importance Sampling methods within DAKOTA.

The NonDAdaptImpSampling implements the multi-modal adaptive importance sampling used for reliability calculations. (eventually we will want to broaden this). Need to add more detail to this description.
13.94.2 Constructor & Destructor Documentation

NonDAdaptImpSampling (ProblemDescDB & problem_db, Model & model)

standard constructor

This is the primary constructor. It accepts a Model reference. It will perform refinement for all response QOI and all probability levels.

References Dakota::abort_handler(), ProblemDescDB::get_iv(), NonD::initialize_random_variables(), Iterator::iteratedModel, NonDSampling::numSamples, Iterator::probDescDB, NonDAdaptImpSampling::refineSamples, NonDSampling::sampleType, NonDSampling::statsFlag, NonD::transform_model(), NonDAdaptImpSampling::useModelBounds, and NonDAdaptImpSampling::uSpaceModel.

NonDAdaptImpSampling (Model & model, unsigned short sample_type, int refine_samples, int refine_seed, const String & rng, bool vary_pattern, unsigned short is_type, bool cdf_flag, bool x_space_model, bool use_model_bounds, bool track_extreme)

alternate constructor for on-the-fly instantiations

This is an alternate constructor for instantiations on the fly using a Model but no ProblemDescDB. It will perform refinement for one response QOI and one probability level (passed in initialize()).

References NonD::cdfFlag, NonDSampling::extremeValues, Iterator::maxEvalConcurrency, Analyzer::numFunctions, NonDAdaptImpSampling::refineSamples, NonDAdaptImpSampling::trackExtremeValues, NonD::transform_model(), NonDAdaptImpSampling::useModelBounds, and NonDAdaptImpSampling::uSpaceModel.

13.94.3 Member Function Documentation

void initialize (const RealVectorArray & acv_points, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)

initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations

Initializes data using a vector array of starting points.

References NonDAdaptImpSampling::designPoint, NonDAdaptImpSampling::failThresh, NonDAdaptImpSampling::initPointsU, NonDAdaptImpSampling::invertProb, NonD::natafTransform, NonD::numContDesVars, NonD::numUncertainVars, NonDAdaptImpSampling::probEstimate, and NonDAdaptImpSampling::respFnIndex.

Referenced by NonDExpansion::compute_numerical_stat_refinements(), NonDAdaptImpSampling::core_run(), and NonDGlobalReliability::importance_sampling().

void initialize (const RealMatrix & acv_points, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)

initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations

Initializes data using a matrix of starting points.

References NonDAdaptImpSampling::designPoint, NonDAdaptImpSampling::failThresh, NonDAdaptImpSampling::initPointsU, NonDAdaptImpSampling::invertProb, NonD::natafTransform, NonD::numContDesVars, NonD::numUncertainVars, NonDAdaptImpSampling::probEstimate, and NonDAdaptImpSampling::respFnIndex.
void initialize ( const RealVector & acv_point, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold )

initializes data needed for importance sampling: an initial point around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations.

Initializes data using only one starting point.

References NonDAadaptImpSampling::designPoint, NonDAadaptImpSampling::failThresh, NonDAadaptImpSampling::initPointsU, NonDAadaptImpSampling::invertProb, NonD::natafTransform, NonD::numContDesVars, NonD::numUncertainVars, NonDAadaptImpSampling::probEstimate, and NonDAadaptImpSampling::respFnIndex.

The documentation for this class was generated from the following files:

- NonDAadaptImpSampling.hpp
- NonDAadaptImpSampling.cpp

13.95 NonDAadaptiveSampling Class Reference

Class for testing various Adaptively sampling methods using geometric, statistical, and topological information of the surrogate.

Inheritance diagram for NonDAadaptiveSampling:

```
NonDAadaptiveSampling
  NonDSampling
    NonD
      Analyzer
        Iterator
```

Public Member Functions

- NonDAadaptiveSampling (ProblemDescDB &problem_db, Model &model)
  _stdarad constructor_

- ~NonDAadaptiveSampling ()
  _alternate constructor for sample generation and evaluation “on the fly” has not been implemented_

- bool resize ()
  _reinitializes iterator based on new variable size_

Protected Member Functions

- void derived_init_communicators (ParLevIter p_iter)
  _derived class contributions to initializing the communicators associated with this Iterator instance_

- void derived_set_communicators (ParLevIter p_iter)
derived class contributions to setting the communicators associated with this Iterator instance

• void derived_free_communicators (ParLevLIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance

• void core_run ()
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

• Real final_probability ()
• void print_results (std::ostream &s)
  print the final iterator results

Private Member Functions

• void calc_score_alm ()
  Function to compute the ALM scores for the candidate points ALM score is the variance computed by the surrogate
  at the point.

• void calc_score_delta_x ()
  Function to compute the Distance scores for the candidate points Distance score is the shortest distance between
  the candidate and an existing training point.

• void calc_score_delta_y ()
  Function to compute the Gradient scores for the candidate points Gradient score is the function value difference
  between a candidate’s surrogate response and its nearest evaluated true response from the training set.

• void calc_score_topo_bottleneck ()
  Function to compute the Bottleneck scores for the candidate points Bottleneck score is computed by determining the
  bottleneck distance between the persistence diagrams of two approximate Morse-Smale complices. The complices
  used include one built from only the training data, and another built from the training data and the single candidate.

• void calc_score_topo_avg_persistence (int respFnCount)
  Function to compute the Average Change in Persistence scores for the candidate points Avg Persistence score is computed
  as the average change in persistence each point undergoes between two approximate Morse-Smale complices. The complices
  used include one built from only the training data, and another built from the training data and the single candidate.

• void calc_score_topo_highest_persistence (int respFnCount)
  Function to compute the Highest Persistence scores for the candidate points Highest Persistence score is calculated
  as a ranking of a set of candidates by constructing an approximate Morse-Smale complex over the entire set of candidates,
  using their surrogate responses, and the training data, using their true responses, and ranking points based on the most
topological significance as measured by their persistence values. In the case where there are no
topologically significant points, the point will be chosen randomly TODO: It may be wiser to fall back to a scheme
that ranks points based on proximity to extrema, or the most significant extream?

• void calc_score_topo_alm_hybrid (int respFnCount)
  Function to compute the Hybrid scores for the candidate points Hybrid score is computed the same as Avg Persistence
  score except that instead of computing one score, three scores are computing not only a mean surface, but a mean +/- std. dev.
surfaces and then averaging the three separate scores. The hope is that you strike a balance between selecting points in topologically important areas and areas of high uncertainty.

• Real calc_score_alm (int respFnCount, RealVector &test_point)
  Same as the other function of the same name, only this allows the user to specify the location of the candidate.

• Real calc_score_delta_x (int respFnCount, RealVector &test_point)
  Same as the other function of the same name, only this allows the user to specify the location of the candidate.

• Real calc_score_delta_y (int respFnCount, RealVector &test_point)
  Same as the other function of the same name, only this allows the user to specify the location of the candidate.
• Real **calc_score_topo_bottleneck** (int respFnCount, RealVector &test_point)
  
  *Same as the other function of the same name, only this allows the user to specify the location of the candidate.*

• Real **calc_score_topo_avg_persistence** (int respFnCount, RealVector &test_point)

  *Same as the other function of the same name, only this allows the user to specify the location of the candidate.*

• Real **calc_score_topo_alm_hybrid** (int respFnCount, RealVector &test_point)

  *Same as the other function of the same name, only this allows the user to specify the location of the candidate.*

• Real **compute_rmspe ()**

  *Using the validationSet, compute the RMSE over the surface.*

• void **compare_complces** (int dim, std::ostream &output)

  *Using the validationSet, compute the approximate Morse-Smale complexes of the true model over the validationSet as well as the surrogate model over the validationSet, and output some topological comparisons.*

• void **parse_options ()**

  *Parse misc options specified in a user input deck.*

• RealVectorArray **drawNewX** (int this_k, int respFnCount=0)

  *function to pick the next X value to be evaluated by the Iterated model*

• void **output_round_data** (int round, int respFnCount=0)

  *Temporary function for dumping validation data to output files to be visualized in TopoAS.*

• void **update_amsce** (int respFnCount=0)

  *Update the approximate Morse-Smale complex based on the training points and selected candidates. Uses surrogate function responses.*

• void **construct_fsu_sampler** (Iterator &u_space_sampler, Model &u_model, int num_samples, int seed, unsigned short sample_type)

  *Copy of construct_lhs only it allows for the construction of FSU sample designs. This can break the fsu_cvt, so it is not used at the moment, and these designs only affect the initial sample build not the candidate sets constructed at each round.*

• void **output_for_optimization** (int dim)

  *This function will write an input deck for a multi-start global optimization run of DAKOTA by extracting all of the local minima off the approximate Morse-Smale complex created from the validation set of the surrogate model.*

• Real **median** (const RealVector &sorted_data)

  *compute the median of the sorted values passed in*

• void **pick_new_candidates ()**

  *Pick new candidates from Emulator.*

• void **score_new_candidates ()**

  *Score New candidates based on the chosen metrics.*

**Private Attributes**

• **Iterator gpBuild**

  *LHS iterator for building the initial GP.*

• **Iterator gpEval**

  *LHS iterator for sampling on the GP.*

• **Iterator gpFinalEval**

  *LHS iterator for sampling on the final GP.*

• **Model gpModel**
GP model of response, one approximation per response function.

- int numRounds
  the number of rounds of additions of size batchSize to add to the original set of LHS samples

- int numPtsTotal
  the total number of points

- int numEmulEval
  the number of points evaluated by the GP each iteration

- int numFinalEmulEval
  number of points evaluated on the final GP

- int scoringMethod
  the type of scoring metric to use for sampling

- Real finalProb
  the final calculated probability (p)

- RealVectorArray gpCvars
  Vector to hold the current values of the current sample inputs on the GP.

- RealVectorArray gpMeans
  Vector to hold the current values of the current mean estimates for the sample values on the GP.

- RealVectorArray gpVar
  Vector to hold the current values of the current variance estimates for the sample values on the GP.

- RealVector emulEvalScores
  Vector to hold the scored values for the current GP samples.

- RealVector predictionErrors
  Vector to hold the RMSE after each round of adaptively fitting the model.

- RealVectorArray validationSet
  Validation point set used to determine predictionErrors above.

- RealVector yTrue
  True function responses at the values corresponding to validationSet.

- RealVector yModel
  Surrogate function responses at the values corresponding to validationSet.

- int validationSetSize
  Number of points used in the validationSet.

- int batchSize
  Number of points to add each round, default = 1.

- String batchStrategy
  String describing the type of batch addition to use. Allowable values are naive, distance, topology.

- String outputDir
  Temporary string for dumping validation files used in TopoAS visualization.

- String scoringMetric
  String describing the method for scoring candidate points. Options are: alm, distance, gradient, highest_persistence, avg_persistence, bottleneck, alm_topo_hybrid. Note: alm and alm_topo_hybrid will fail when used with surrogates other than global_kriging as it is based on the variance of the surrogate. At the time of implementation, global_kriging is the only surrogate capable of yielding this information.

- unsigned short sampleDesign
enum describing the initial sample design. Options are: RANDOM_SAMPLING, FSU_CVT, FSU_HALTON, FSU_HAMMERSLEY

- String approx_type
  
  String describing type of surrogate is used to fit the data. Options are: global_kriging, global_mars, global_neural_network, global_polynomial, global_moving_least_squares, global_radial_basis.

- MS_Complex * AMSC
  
  The approximate Morse-Smale complex data structure.

- int numKneighbors
  
  The number of approximate nearest neighbors to use in computing the AMSC.

- bool outputValidationData
  
  Temporary variable for toggling writing of data files to be used by TopoAS.

### Additional Inherited Members

#### 13.95.1 Detailed Description

Class for testing various Adaptively sampling methods using geometric, statistical, and topological information of the surrogate.

**NonDAdaptiveSampling** implements an adaptive sampling method based on the work presented in Adaptive Sampling with Topological Scores by Dan Maljovec, Bei Wang, Ana Kupresanin, Gardar Johannesson, Valerio Pascucci, and Peer-Timo Bremer presented in IJUQ (insert issue). The method computes scores based on the topology of the known data and the topology of the surrogate model. A number of alternate adaption strategies are offered as well.

#### 13.95.2 Constructor & Destructor Documentation

NonDAdaptiveSampling ( ProblemDescDB & problem_db, Model & model )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), Response::active_set(), NonDAdaptiveSampling::AMSC, NonDAdaptiveSampling::approx_type, Iterator::assign_rep(), Model::assign_rep(), NonDAdaptiveSampling::batchSize, NonDAdaptiveSampling::batchStrategy, NonDAdaptiveSampling::construct_fsu_sampler(), NonD::construct_lhs(), Model::current_response(), ProblemDescDB::getBool(), ProblemDescDB::getInt(), ProblemDescDB::getIv(), ProblemDescDB::getSa(), ProblemDescDB::getString(), ProblemDescDB::getUshort(), NonDAdaptiveSampling::gpBuild, NonDAdaptiveSampling::gpEval, NonDAdaptiveSampling::gpFinalEval, NonDAdaptiveSampling::gpModel, Model::gradient_type(), Model::hessian_type(), Iterator::iteratedModel, Iterator::maxIterations, NonDAdaptiveSampling::numEmulEval, NonDAdaptiveSampling::numFinalEmulEval, NonDAdaptiveSampling::numKneighbors, NonDAdaptiveSampling::numRounds, NonDSampling::numSamples, NonDAdaptiveSampling::outputDir, Iterator::outputLevel, NonDAdaptiveSampling::outputValidationData, NonDAdaptiveSampling::parse_options(), Iterator::probDescDB, NonDSampling::randomSeed, ActiveSet::request_values(), NonDSampling::rngName, NonDAdaptiveSampling::sampleDesign, NonDSampling::sampleType, NonDAdaptiveSampling::scoringMetric, NonDSampling::vary_pattern(), and NonDSampling::varyPattern.
 alternate constructor for sample generation and evaluation "on the fly" has not been implemented destructor

13.95.3 Member Function Documentation

void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Iterator::all_responses(), Model::append_approximation(), Model::approximation_data(), NonDAdaptiveSampling::batchSize, Model::build_approximation(), NonDAdaptiveSampling::compare_complices(), NonDAdaptiveSampling::compute_rmspe(), Non::computedProbLevels, Model::continuous_variables(), Model::current_variables(), NonDAdaptiveSampling::drawNewX(), Model::evaluate(), Model::evaluation_id(), NonDAdaptiveSampling::gpCvars, NonDAdaptiveSampling::gpFinalEval, NonDAdaptiveSampling::gpMeans, NonDAdaptiveSampling::gpModel, NonDAdaptiveSampling::gpVar, NonD::initialize_level_mappings(), Iterator::iteratedModel, Iterator::methodPCIter, NonD::miPLIndex, NonDAdaptiveSampling::numEmulEval, NonDAdaptiveSampling::numFinalEmulEval, Analyzer::numFunctions, NonDAdaptiveSampling::numPtsTotal, NonDAdaptiveSampling::numRounds, NonD::numSamples, NonDAdaptiveSampling::output_round_data(), NonDAdaptiveSampling::pick_new_candidates(), NonDAdaptiveSampling::predictionErrors, NonD::requestedRespLevels, Iterator::run(), NonDAdaptiveSampling::score_new_candidates(), NonDAdaptiveSampling::scoringMetric, and NonDAdaptiveSampling::update_amsc().

void print_results ( std::ostream & s ) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References NonD::print_level_mappings(), and NonD::statsFlag.

The documentation for this class was generated from the following files:

- NonDAdaptiveSampling.hpp
- NonDAdaptiveSampling.cpp

13.96 NonDBayesCalibration Class Reference

Base class for Bayesian inference: generates posterior distribution on model parameters given experimental data.

Inheritance diagram for NonDBayesCalibration:
Public Member Functions

- **NonDBayesCalibration** (ProblemDescDB &problem_db, Model &model)  
  *standard constructor*

- ~**NonDBayesCalibration** ()  
  *destructor*

- template<typename VectorType> 
  Real **prior_density** (const VectorType &vec)  
  *compute the prior PDF for a particular MCMC sample*

- template<typename VectorType> 
  Real **log_prior_density** (const VectorType &vec)  
  *compute the log prior PDF for a particular MCMC sample*

- template<typename Engine> 
  void **prior_sample** (Engine &rng, RealVector &prior_samples)  
  *draw a multivariate sample from the prior distribution*

- template<typename VectorType> 
  void **prior_mean** (VectorType &mean_vec) const  
  *return the mean of the prior distribution*

- template<typename MatrixType> 
  void **prior_variance** (MatrixType &var_mat) const  
  *return the covariance of the prior distribution*

Static Public Member Functions

- static void **get_positive_definite_covariance_from_hessian** (const RealSymMatrix &hessian, const RealMatrix &prior_chol_fact, RealSymMatrix &covariance, short output_lev)  
  *Compute the proposal covariance C based on low-rank approximation to the prior-preconditioned misfit Hessian.*

- static Real **knn_kl_div** (RealMatrix &distX_samples, RealMatrix &distY_samples, size_t dim)

- static Real **knn_mutual_info** (RealMatrix &Xmatrix, int dimX, int dimY)
Protected Member Functions

- void 
  core_run ()
  
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

- void 
  derived_init_communicators (ParLevLIter pl_iter)
  
  derived class contributions to initializing the communicators associated with this Iterator instance

- void 
  derived_set_communicators (ParLevLIter pl_iter)
  
  derived class contributions to setting the communicators associated with this Iterator instance

- void 
  derived_free_communicators (ParLevLIter pl_iter)
  
  derived class contributions to freeing the communicators associated with this Iterator instance

- void 
  print_results (std::ostream &s)
  
  print the final iterator results

- const Model & 
  algorithm_space_model () const

- virtual void 
  calibrate ()=0
  
  Perform Bayesian calibration (all derived classes must implement)

- void 
  construct_mcmc_model ()
  
  construct mcmcModel (no emulation, GP, PCE, or SC) that wraps inbound Model

- void 
  init_hyper_parameters ()
  
  initialize the hyper-parameter priors

- void 
  construct_map_optimizer ()
  
  construct the negative log posterior RecastModel (wraps residualModel) and corresponding MAP optimizer

- void 
  initialize_model ()
  
  initialize emulator model and probability space transformations

- void 
  calibrate_to_hifi ()
  
  calibrate the model to a high-fidelity data source, using mutual information-guided design of experiments (adaptive experimental design)

- void 
  build_model_discrepancy ()
  
  calculate model discrepancy with respect to experimental data

- void 
  extract_selected_posterior_samples (const std::vector< int > &points_to_keep, const RealMatrix &samples_for_posterior_eval, const RealVector &posterior_density, RealMatrix &posterior_data) const

- void 
  export_posterior_samples_to_file (const std::string filename, const RealMatrix &posterior_data) const

- template<typename VectorType1 , typename VectorType2 >
  void 
  augment_gradient_with_log_prior (VectorType1 &log_grad, const VectorType2 &vec)
  
  compute the (approximate) gradient of the negative log posterior by augmenting the (approximate) gradient of the negative log likelihood with the gradient of the negative log prior

- template<typename MatrixType , typename VectorType >
  void 
  augment_hessian_with_log_prior (MatrixType &log_hess, const VectorType &vec)
  
  compute the (approximate) Hessian of the negative log posterior by augmenting the (approximate) Hessian of the negative log likelihood with the Hessian of the negative log prior

- Real 
  log_likelihood (const RealVector &residuals, const RealVector &hyper_params)
  
  calculate log-likelihood from the passed residuals (assuming they are already sized and scaled by covariance / hyperparams...)

- void 
  prior_cholesky_factorization ()
  
  compute priorCovCholFactor based on prior distributions for random variables and any hyperparameters
- void `get_positive_definite_covariance_from_hessian` (const RealSymMatrix &hessian, RealSymMatrix &covariance)
  member version forwards member data to static function
- void `export_discrepancy` (RealMatrix &pred_config_mat)
  print tabular files containing model+discrepancy responses and variances
- void `compute_statistics` ()
  Compute final stats for MCMC chains.
- void `export_chain` ()
  export the acceptance chain in user space
- void `export_chain` (RealMatrix &filtered_chain, RealMatrix &filtered_fn_vals)
  Print filtered posterior and function values (later: credibility and prediction intervals)
- void `filter_chain` (RealMatrix &acceptance_chain, RealMatrix &filtered_chain)
  Perform chain filtering with burn-in and sub-sampling.
- void `filter_fnvals` (RealMatrix &accepted_fn_vals, RealMatrix &filtered_fn_vals)
- void `compute_intervals` ()
- void `compute_prediction_vals` (RealMatrix &filtered_fn_vals, RealMatrix &PredVals, int num_filtered, size_t num_exp, size_t num_concatenated)
- void `compute_col_means` (RealMatrix &matrix, RealVector &avg_vals)
- void `compute_col_stdevs` (RealMatrix &matrix, RealVector &avg_vals, RealVector &std_devs)
- void `print_intervals_file` (std::ostream &stream, RealMatrix &functionvalsT, RealMatrix &predvalsT, int length, size_t aug_length)
- void `print_intervals_screen` (std::ostream &stream, RealMatrix &functionvalsT, RealMatrix &predvalsT, int length)
- void `kl_post_prior` (RealMatrix &acceptanceChain)
  Compute information metrics.
- void `prior_sample_matrix` (RealMatrix &prior_dist_samples)
- void `mutual_info_buildX` ()
- void `print_kl` (std::ostream &stream)

Static Protected Member Functions

- static void `neg_log_post_resp_mapping` (const Variables &model_vars, const Variables &nlpost_vars, const Response &model_resp, Response &nlpost_resp)
  static function passed by pointer to negLogPostModel recast model
- static void `ann_dist` (const ANNpointArray matrix1, const ANNpointArray matrix2, RealVector &distances, int NX, int NY, int dim2, IntVector &k, double eps)

Protected Attributes

- String `scalarDataFilename`
- short `emulatorType`
  the emulator type: NO_EMULATOR, GP_EMULATOR, PCE_EMULATOR, or SC_EMULATOR
- Model `mcmcModel`
  `Model` instance employed in the likelihood function; provides response function values from Gaussian processes, stochastic expansions (PCE/SC), or direct access to simulations (no surrogate option)
- bool `mcmcModelHasSurrogate`
whether the MCMC Model is a surrogate, or a thin transformation around a surrogate, so can be cheaply re-evaluated in chain recovery

- **Model residualModel**
  DataTransformModel wrapping the mcmcModel.

- **Iterator mapOptimizer**
  SQP or NIP optimizer for pre-solving for the MAP point prior to MCMC. This is restricted to emulator cases for now, but as for derivative preconditioning, could be activated for no-emulator cases with a specification option (not active by default).

- **Model negLogPostModel**
  RecastModel for solving for MAP: reduces residualModel to scalar negative log posterior.

- **unsigned short mapOptAlgOverride**
  user setting of the MAP optimization algorithm type

- **Iterator stochExpIterator**
  NonDPolynomialChaos or NonDStochCollocation instance for defining a PCE/SC-based mcmcModel.

- **int chainSamples**
  number of samples in the chain (e.g. number of MCMC samples); for iterative update cycles, number of samples per update cycle

- **int chainCycles**
  number of update cycles for MCMC chain (implemented by restarting of short chains)

- **int randomSeed**
  random seed for MCMC process

- **short mcmcDerivOrder**
  order of derivatives used in MCMC process (bitwise like ASV)

- **bool adaptExpDesign**
  whether to perform iterative design of experiments with high-fidelity model

- **size_t numCandidates**
  number of candidate designs for adaptive Bayesian experimental design

- **String importCandPtsFile**
  whether to import candidate design points for adaptive Bayesian experimental design

- **unsigned short importCandFormat**
  tabular format for the candidate design points import file

- **int maxHifiEvals**
  maximum number of high-fidelity model runs to be used for adaptive Bayesian experimental design

- **bool calModelDiscrepancy**
  flag whether to calculate model discrepancy

- **String discrepancyType**
  set discrepancy type

- **String exportCorrModelFile**
  filename for corrected model (model+discrepancy) calculations output

- **String exportDiscrepFile**
  filename for discrepancy calculations output

- **String exportCorrVarFile**
  filename for corrected model variance calculations

- **unsigned short exportCorrModelFormat**
format options for corrected model output

- unsigned short exportDiscrepFormat
  format options for discrepancy output
- unsigned short exportCorrVarFormat
  format options for corrected model variance output
- short approxCorrectionOrder
  specify polynomial or trend order for discrepancy correction
- size_t numPredConfigs
  number of prediction configurations at which to calculate model discrepancy

- RealVector configLowerBnds
  lower bounds on configuration domain
- RealVector configUpperBnds
  upper bounds on configuration domain
- ResponseArray discrepancyResponses
  array containing predicted of model+discrepancy
- ResponseArray correctedResponses
  array containing predicted of model+discrepancy
- RealMatrix correctedVariances
  matrix containing variances of model+discrepancy
- RealVector predictionConfigList
  list of prediction configurations at which to calculate model discrepancy
- String importPredConfigs
  whether to import prediction configurations at which to calculate model discrepancy
- unsigned short importPredConfigFormat
  tabular format for prediction configurations import file
- Model hifiModel
  a high-fidelity model data source (given by pointer in input)
- int initHifiSamples
  initial high-fidelity model samples
- Iterator hifiSampler
  LHS iterator to generate hi-fi model data.
- RealMatrix priorCovCholFactor
  the Cholesky factor of the prior covariance
- unsigned short obsErrorMultiplierMode
  mode for number of observation error multipliers to calibrate (default none)
- int numHyperparams
  calculated number of hyperparameters augmenting the calibration parameter set, e.g., due to calibrate observation error multipliers
- RealVector invGammaAlphas
  alphas for inverse gamma distribution on hyper-params
- RealVector invGammaBetass
  alphas for inverse gamma distribution on hyper-params
• `std::vector<Pecos::RandomVariable>` invGammaDists
  distributions for hyper-params
• `bool` standardizedSpace
  flag indicating use of a variable transformation to standardized probability space for the model or emulator
• `bool` posteriorStatsKL
  flag indicating the calculation of KL divergence between prior and posterior
• `bool` posteriorStatsMutual
  flag indicating the calculation of mutual information between prior and posterior
• `bool` adaptPosteriorRefine
  flag indicating usage of adaptive posterior refinement; currently makes sense for unstructured grids in GP and PCE least squares/CS
• `String` proposalCovarType
  approach for defining proposal covariance
• `RealVector` proposalCovarData
  data from user input of proposal covariance
• `String` proposalCovarFilename
  filename for user-specified proposal covariance
• `String` proposalCovarInputType
  approach for defining proposal covariance
• `RealMatrix` acceptanceChain
  Post-processing-related controls.
• `RealMatrix` acceptedFnVals
  cached function values corresponding to acceptanceChain for final statistics reporting
• `std::map<Real, RealVector>` bestSamples
  container for managing best MCMC samples (points and associated log posterior) collected across multiple (restarted) chains
• `int` burnInSamples
  number of MCMC samples to discard from acceptance chain
• `int` subSamplingPeriod
  period or skip in post-processing the acceptance chain
• `RealMatrix` chainStats
• `RealMatrix` fnStats
• `RealMatrix` predVals
  Compute credibility and prediction intervals of final chain.
• `RealMatrix` filteredFnVals
  cached filtered function values for printing
• `String` exportMCMCFilename
  output filename for the MCMC chain
• `short` exportMCMCFormat
  output formatting options for MCMC export
• `short` filteredMCMCFormat
• `Real` kl_est
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Static Protected Attributes

- static NonDBayesCalibration * nonDBayesInstance
  Pointer to current class instance for use in static callback functions.

13.96.1 Detailed Description

Base class for Bayesian inference: generates posterior distribution on model parameters given experimental data.

This class will eventually provide a general-purpose framework for Bayesian inference. In the short term, it only collects shared code between QUESO and GPMSA implementations.

13.96.2 Constructor & Destructor Documentation

NonDBayesCalibration ( ProblemDescDB & probDB, Model & model )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDBayesCalibration::adaptExpDesign, NonDBayesCalibration::adaptPosteriorRefine, Iterator::assign_rep(), Model::assign_rep(), NonDCalibration::calibrationData, NonDBayesCalibration::chainCycles, NonDBayesCalibration::chainSamples, NonDBayesCalibration::construct_map_optimizer(), NonDBayesCalibration::construct_mcmc_model(), Model::continuous_lower_bound(), Model::continuous_upper_bound(), NonDBayesCalibration::emulatorType, NonDCalibration::expData, NonD::generate_system_seed(), ProblemDescDB::get_bool(), ProblemDescDB::get_int(), NonDBayesCalibration::hifiModel, NonDBayesCalibration::hifiSampler, NonDBayesCalibration::init_hyper_parameters(), NonDBayesCalibration::initHifiSamples, NonD::initialize_random_variable_correlations(), NonD::initialize_random_variable_transformation(), NonD::initialize_random_variable_types(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, Iterator::maxIterations, NonDBayesCalibration::mcmcModel, Model::model_type(), ExperimentData::num_experiments(), Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, NonDBayesCalibration::obsErrorMultiplierMode, Iterator::probDescDB, NonDBayesCalibration::proposalCovarType, NonDBayesCalibration::randomSeed, NonDBayesCalibration::residualModel, NonDBayesCalibration::standardizedSpace, Model::truth_model(), Analyzer::vary_pattern(), and NonD::verify_correlation_support().

13.96.3 Member Function Documentation

void prior_mean ( VectorType & mean_vec ) const

return the mean of the prior distribution

Assume the target mean_vec is sized by client

References NonDBayesCalibration::invGammaDists, NonD::natafTransform, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, and NonDBayesCalibration::standardizedSpace.

void prior_variance ( MatrixType & var_mat ) const

return the covariance of the prior distribution

Assume the target var_mat is sized by client

References NonDBayesCalibration::invGammaDists, NonD::natafTransform, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, and NonDBayesCalibration::standardizedSpace.
CHAPTER 13. CLASS DOCUMENTATION

void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
  Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
  Reimplemented from Iterator.
  References NonDBayesCalibration::adaptExpDesign, NonDBayesCalibration::build_model_discrepancy(), Non-
  DBayesCalibration::calibrate(), NonDBayesCalibration::calibrate_to_hifi(), NonDBayesCalibration::calModelDiscrepancy, and
  NonDBayesCalibration::nonDBayesInstance.

void print_results ( std::ostream & s ) [protected], [virtual]

print the final iterator results
  This virtual function provides additional iterator-specific final results outputs beyond the function evaluation
  summary printed in finalize_run().
  Reimplemented from Analyzer.
  Reimplemented in NonDGPMSABayesCalibration, NonDDREAMBayesCalibration, NonDWASABIBayes-
  Calibration, and NonDQUESTOBayesCalibration.
  References Model::continuous_variable_labels(), Dakota::copy_data(), Model::current_response(), NonDBayes-
  Calibration::filteredFnVals, Response::function_labels(), NonDBayesCalibration::mcmcModel, NonDBayesCalibration-
  ::posteriorStatsKL, NonDSampling::print_moments(), and NonDBayesCalibration::residualModel.
  Referenced by NonDQUESOBayesCalibration::print_results(), NonDWASABIBayesCalibration::print_results(), Non-
  DDREAMBayesCalibration::print_results(), and NonDGPMSABayesCalibration::print_results().

const Model & algorithm_space_model ( ) const [inline], [protected], [virtual]

default definition that gets redefined in selected derived Minimizers
  Reimplemented from Analyzer.
  References NonDBayesCalibration::mcmcModel.

void construct_map_optimizer ( ) [protected]

construct the negative log posterior RecastModel (wraps residualModel) and corresponding MAP optimizer
  Construct optimizer for MAP pre-solve Emulator: on by default; can be overridden with "pre_solve none" No
  emulator: off by default; can be activated with "pre_solve {sqp,nip}" relies on mapOptimizer ctor to enforce min
  derivative support
  References Iterator::assign_rep(), Model::assign_rep(), Iterator::convergenceTol, NonDBayesCalibration::emulator-
  Type, Iterator::gnewton_set_recast(), NonDBayesCalibration::mapOptAlgOverride, NonDBayesCalibration::map-
  Optimizer, NonDBayesCalibration::mcmcDerivOrder, NonDBayesCalibration::neg_log_post_resp_mapping(), Non-
  DBayesCalibration::negLogPostModel, Model::num_primary_fns(), and NonDBayesCalibration::residualModel.
  Referenced by NonDBayesCalibration::calibrate_to_hifi(), and NonDBayesCalibration::NonDBayesCalibration().

Real log_likelhood ( const RealVector & residuals, const RealVector & all_params ) [protected]

calculate log-likelihood from the passed residuals (assuming they are already sized and scaled by covariance /
  hyperparams...
  Calculate the log-likelihood, accounting for contributions from covariance and hyperparameters, as well as
  constant term:
    \[ \log(L) = -1/2\times Nr\times \log(2\times \pi) - 1/2\times \log(\det(Cov)) - 1/2\times r'(Cov^{-1})\times r \]
  The passed residuals must already be size-adjusted, differenced with any data, if present, and scaled by
  covariance^{-1/2}.
References NonDCalibration::expData, Dakota::HALF_LOG_2PI, ExperimentData::half_log_cov_determinant(), Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, and NonDBayesCalibration::obsErrorMultiplierMode.

Referenced by NonDQUESOBayesCalibration::dakotaLogLikelihood(), NonDBayesCalibration::neg_log_postresp_mapping(), and NonDDREAMBayesCalibration::sample_likelihood().

```c++
void neg_log_postresp_mapping ( const Variables & residual_vars, const Variables & nlpost_vars, const Response & residual_resp, Response & nlpost_resp ) [static], [protected]
static function passed by pointer to negLogPostModel recast model
    Response mapping callback used within RecastModel for MAP pre-solve. Computes
    -log(post) = -log(like) - log(prior); where -log(like) = 1/2*Nr*log(2*pi) + 1/2*log(det(Cov)) + 1/2*r'(Cov^\{-1\})r
    = 1/2*Nr*log(2*pi) + 1/2*log(det(Cov)) + misfit
    (misfit defined as 1/2 r^T (multi^\{-2\}Gamma_d)\{\{-1\} r) The passed residual_resp has been differenced, interpolated, and covariance-scaled
References Response::active_set_request_vector(), NonDBayesCalibration::augment_gradient_with_log_prior(), NonDBayesCalibration::augment_hessian_with_log_prior(), ExperimentData::build_gradient_of_sum_square_residuals(), ExperimentData::build_hessian_of_sum_square_residuals(), Variables::continuous_variables(), NonDCalibration::expData, Response::function_gradient_view(), Response::function_hessian_view(), Response::function_value(), Response::function_values(), ExperimentData::half_log_cov_det_gradient(), ExperimentData::half_log_cov_det_hessian(), NonDBayesCalibration::loglikelihood(), NonDBayesCalibration::log_prior_density(), NonDBayesCalibration::nonDBayesInstance, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, NonDBayesCalibration::obsErrorMultiplierMode, and Iterator::outputLevel.
Referenced by NonDBayesCalibration::construct_map_optimizer().
```

```c++
void export_chain ( RealMatrix & filtered_chain, RealMatrix & filtered_fn_vals ) [protected]
Print filtered posterior and function values (later: credibility and prediction intervals)
    Print tabular file with filtered chain, function values, and pred values
References Variables::continuous_variables(), Variables::copy(), Model::current_response(), Model::current_variables(), NonDBayesCalibration::exportMCMCFilename, NonDBayesCalibration::exportMCMCFormat, Response::function_labels(), Model::interface_id(), NonDBayesCalibration::mcmcModel, Analyzer::numFunctions, NonDBayesCalibration::residualModel, Dakota::write_precision, and Variables::write_tabular().
```

### 13.96.4 Member Data Documentation

**RealMatrix acceptanceChain [protected]**

Post-processing-related controls.
- accumulation of acceptance chain across restarts (stored in user-space) TO DO: retire once restarts are retired; optimize to convert to user-space only in final results

Referenced by NonDQUESOBayesCalibration::aggregate_acceptance_chain(), NonDDREAMBayesCalibration::archive_acceptance_chain(), NonDDREAMBayesCalibration::archive_acceptance_chain(), NonDBayesCalibration::build_model_discrepancy(), NonDGPMSABayesCalibration::cache_acceptance_chain(), NonDDREAMBayesCalibration::cache_chain(), NonDBayesCalibration::calibrate_to_hifi(), NonDBayesCalibration::compute_statistics(), and NonDQUESOBayesCalibration::run_chain_with_restarting().

The documentation for this class was generated from the following files:
- NonDBayesCalibration.hpp
- NonDBayesCalibration.cpp
13.97 NonDCalibration Class Reference

Inheritance diagram for NonDCalibration:

```
    Iterator
       |    
    Analyzer
       |    
    NonD
       |    
NonDCalibration
       |    
    NonDBayesCalibration
       |    
  NonDDREAMBayesCalibration  NonDQUESOBayesCalibration  NonDWASABIBayesCalibration
       |    
NonDGPMSEBayesCalibration
```

Public Member Functions

- **NonDCalibration** (ProblemDescDB &problem_db, Model &model)
  
  *standard constructor*

- **~NonDCalibration** ()
  
  *destructor*

- **bool resize ()**
  
  *reinitializes iterator based on new variable size*

Protected Attributes

- **bool calibrationData**
  
  *flag indicating whether there is calibration data present*

- **ExperimentData expData**
  
  *Container for experimental data to which to calibrate model.*

Additional Inherited Members

13.97.1 Detailed Description

This class ...

13.97.2 Constructor & Destructor Documentation

NonDCalibration (ProblemDescDB &problem_db, Model &model)

*standard constructor*
This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References NonDCalibration::calibrationData, NonDCalibration::expData, ExperimentData::load_data(), and Iterator::outputLevel.

The documentation for this class was generated from the following files:

- NonDCalibration.hpp
- NonDCalibration.cpp

### 13.98 NonDCubature Class Reference

Derived nondeterministic class that generates N-dimensional numerical cubature points for evaluation of expectation integrals.

Inheritance diagram for NonDCubature:

```
Analyzer
NonD
NonDIntegration
NonDCubature
```

#### Public Member Functions

- **NonDCubature** (Model &model, const Pecos::ShortArray &u_types, unsigned short cub_int_order)
- unsigned short integrand_order () const
  
  ```
  return cubIntOrder
  ```

#### Protected Member Functions

- **NonDCubature** (ProblemDescDB &problem_db, Model &model)
  
  constructor
- **~NonDCubature** ()
  
  destructor
- void initialize_grid (const std::vector<Pecos::BasisPolynomial> &poly_basis)
  
  initialize integration grid by drawing from polynomial basis settings
- void get_parameter_sets (Model &model)
  
  Generate one block of numSamples samples (ndim * num_samples), populating allSamples: ParamStudy is the only class that specializes to use allVariables.
- void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)
- void increment_grid ()
increment SSG level/TPQ order
- void increment_grid_preference (const RealVector &dim_pref)
- int num_samples () const

Private Member Functions
- void check_integration (const Pecos::ShortArray &u_types, const Pecos::AleatoryDistParams &adp)
  verify self-consistency of integration specification
- void increment_reference ()
  increment each cubIntOrderRef entry by 1

Private Attributes
- Pecos::CubatureDriver * cubDriver
  convenience pointer to the numIntDriver representation
- unsigned short cubIntOrderRef
  reference point for Pecos::CubatureDriver::cubIntOrder: the original user specification for the number of Gauss points per dimension, plus any refinements posted by increment_grid()
- unsigned short cubIntRule
  the isotropic cubature integration rule

Additional Inherited Members

13.98.1 Detailed Description
Derived nondeterministic class that generates N-dimensional numerical cubature points for evaluation of expectation integrals.

This class is used by NonDPolynomialChaos, but could also be used for general numerical integration of moments. It employs Stroud cubature rules and extensions by D. Xiu.

13.98.2 Constructor & Destructor Documentation

NonDCubature ( Model & model, const Pecos::ShortArray & u_types, unsigned short cub_int_order )
This alternate constructor is used for on-the-fly generation and evaluation of numerical cubature points.

References Model::aleatory_distribution_parameters(), NonDCubature::check_integration(), NonDCubature::cubDriver, NonDCubature::cubIntOrderRef, Iterator::iteratedModel, and NonDIntegration::numIntDriver.

NonDCubature ( ProblemDescDB & problem_db, Model & model ) [protected]
constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. It is not currently used, as there is not yet a separate nond_cubature method specification.

References Model::aleatory_distribution_parameters(), NonDCubature::check_integration(), NonDIntegration::check_variables(), NonDCubature::cubDriver, NonDCubature::cubIntOrderRef, NonDCubature::cubIntRule, Iterator::iteratedModel, Iterator::maxEvalConcurrency, NonD::natafTransform, and NonDIntegration::numIntDriver.
13.98.3 Member Function Documentation

```cpp
void sampling_reset ( int min_samples, bool all_data_flag, bool stats_flag ) [protected], [virtual]
```

used by DataFitSurrModel::build_global() to publish the minimum number of points needed from the cubature routine in order to build a particular global approximation.

Reimplemented from Iterator.
References NonDCubature::cubDriver, and NonDCubature::cubIntOrderRef.

```cpp
void increment_grid_preference ( const RealVector & dim_pref ) [inline], [protected], [virtual]
```

Should not be used, but pure virtual must be defined.

Reimplemented from NonDIntegration.
References NonDCubature::increment_grid().

```cpp
int num_samples ( ) const [inline], [protected], [virtual]
```

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.
References NonDCubature::cubDriver.

```cpp
void increment_reference ( ) [inline], [private]
```

increment each cubIntOrderRef entry by 1

cubIntOrderRef is a reference point for CubatureDriver::cubIntOrder, e.g., a lower bound

References NonDCubature::cubIntOrderRef.

Referenced by NonDCubature::increment_grid().

The documentation for this class was generated from the following files:

- NonDCubature.hpp
- NonDCubature.cpp

13.99 NonDDREAMBayesCalibration Class Reference

Bayesian inference using the DREAM approach.

Inheritance diagram for NonDDREAMBayesCalibration:
Public Member Functions

- **NonDDREAMBayesCalibration** (ProblemDescDB &problem_db, Model &model)
  
  *standard constructor*

- **~NonDDREAMBayesCalibration** ()
  
  *destructor*

Static Public Member Functions

- static void **problem_size** (int &chain_num, int &cr_num, int &gen_num, int &pair_num, int &par_num)
  
  *initializer for problem size characteristics in DREAM*

- static void **problem_value** (std::string *chain_filename, std::string *gr_filename, double &gr_threshold, int &jumpstep, double limits[], int par_num, int &printstep, std::string *restart_read_filename, std::string *restart_write_filename)
  
  *Filename and data initializer for DREAM.*

- static double **prior_density** (int par_num, double zp[])
  
  *Compute the prior density at specified point zp.*

- static double * **prior_sample** (int par_num)
  
  *Sample the prior and return an array of parameter values.*

- static double **sample_likelihood** (int par_num, double zp[])
  
  *Likelihood function for call-back from DREAM to DAKOTA for evaluation.*

Protected Member Functions

- void **calibrate** ()

- void **print_results** (std::ostream &s)
  
  *print the final iterator results*

- void **archive_acceptance_chain** ()
  
  *save the final x-space acceptance chain and corresponding function values*
Static Protected Member Functions

- static void cache_chain (const double *const z)
  
  Callback to archive the chain from DREAM, potentially leaving it in u-space.

Protected Attributes

- RealVector paramMins
  
  lower bounds on calibrated parameters
- RealVector paramMaxs
  
  upper bounds on calibrated parameters
- int numChains
  
  number of concurrent chains
- int numGenerations
  
  number of generations
- int numCR
  
  number of CR-factors
- int crossoverChainPairs
  
  number of crossover chain pairs
- Real grThreshold
  
  threshold for the Gelman-Rubin statistic
- int jumpStep
  
  how often to perform a long jump in generations
- boost::mt19937 rnumGenerator
  
  random number engine for sampling the prior

Static Private Attributes

- static NonDDREAMBayesCalibration * nonDDREAMInstance
  
  Pointer to current class instance for use in static callback functions.

Additional Inherited Members

13.99.1 Detailed Description

Bayesian inference using the DREAM approach.

This class performed Bayesian calibration using the DREAM (Markov Chain Monte Carlo acceleration by Differential Evolution) implementation of John Burkhardt (FSU), adapted from that of Guannan Zhang (ORNL)

13.99.2 Constructor & Destructor Documentation

NonDDREAMBayesCalibration ( ProblemDescDB & problem_db, Model & model )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References NonDBayesCalibration::chainSamples, NonDDREAMBayesCalibration::crossoverChainPairs, NonDDREAMBayesCalibration::grThreshold, NonDDREAMBayesCalibration::jumpStep, NonDDREAMBayesCalibration::numChains, NonDDREAMBayesCalibration::numCR, and NonDDREAMBayesCalibration::numGenerations.
13.99.3 Member Function Documentation

void problem_size ( int & chain_num, int & cr_num, int & gen_num, int & pair_num, int & par_num )
[static]
initializer for problem size characteristics in DREAM
See documentation in DREAM examples)
References NonDDREAMBayesCalibration::crossoverChainPairs, NonDDREAMBayesCalibration::nonDDREAMInstance, NonDDREAMBayesCalibration::numChains, Analyzer::numContinuousVars, NonDDREAMBayesCalibration::numCR, NonDDREAMBayesCalibration::numGenerations, and NonDBayesCalibration::numHyperparams.

void problem_value ( std::string * chain_filename, std::string * gr_filename, double & gr_threshold, int & jumpstep, double limits[], int par_num, int & printstep, std::string * restart_read_filename, std::string * restart_write_filename )
[static]
Filename and data initializer for DREAM.
See documentation in DREAM examples)
References NonDDREAMBayesCalibration::grThreshold, NonDDREAMBayesCalibration::jumpStep, NonDDREAMBayesCalibration::nonDDREAMInstance, NonDDREAMBayesCalibration::numChains, NonDDREAMBayesCalibration::paramMaxs, and NonDDREAMBayesCalibration::paramMins.

double prior_density ( int par_num, double zp[] )
[static]
Compute the prior density at specified point zp.
See documentation in DREAM examples)
References NonDBayesCalibration::nonDBayesInstance, and NonDBayesCalibration::prior_density().

double * prior_sample ( int par_num )
[static]
Sample the prior and return an array of parameter values.
See documentation in DREAM examples
References NonDBayesCalibration::nonDBayesInstance, NonDDREAMBayesCalibration::nonDDREAMInstance, and NonDDREAMBayesCalibration::numGenerator.

double sample_likelihood ( int par_num, double zp[] )
[static]
Likelihood function for call-back from DREAM to DAKOTA for evaluation.
Static callback function to evaluate the likelihood
References Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_values(), NonDBayesCalibration::log_likelihood(), NonDDREAMBayesCalibration::nonDDREAMInstance, Iterator::outputLevel, and NonDBayesCalibration::residualModel.

void calibrate ()
[protected], [virtual]
Perform the uncertainty quantification DREAM will callback to cache_chain to store the chain
Implements NonDBayesCalibration.
References Dakota::abort_handler(), NonDDREAMBayesCalibration::archive_acceptance_chain(), NonDDREAMBayesCalibration::cache_chain(), NonDCalibration::calibrationData, NonDBayesCalibration::chainSamples,
NonDBayesCalibration::compute_statistics(), Model::continuous_variables(), NonDBayesCalibration::initialize_-
model(), NonDBayesCalibration::mcmcModel, NonD::natafTransform, NonDDREAMBayesCalibration::nonD-
DREAMInstance, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, NonDBayesCalibration-
::obsErrorMultiplierMode, NonDDREAMBayesCalibration::paramMaxs, NonDDREAMBayesCalibration::param-
Mins, NonDBayesCalibration::randomSeed, NonDDREAMBayesCalibration::numGenerator, and NonDBayes-
Calibration::standardizedSpace.

void print_results ( std::ostream & s ) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation
summary printed in finalize.run().

Reimplemented from NonDBayesCalibration.
References NonDBayesCalibration::print_results().

void cache_chain ( const double *const z ) [static], [protected]

Callback to archive the chain from DREAM, potentially leaving it in u-space.

Archive the chain from DREAM. This default implementation is aggregating from the parallel chains in a
round-robin fashion.

References NonDBayesCalibration::acceptanceChain, NonDDREAMBayesCalibration::nonDDREAMInstance,
Analyzer::num_samples(), NonDDREAMBayesCalibration::numChains, Analyzer::numContinuousVars, NonD-
DREAMBayesCalibration::numGenerations, and NonDBayesCalibration::numHyperparams.

Referenced by NonDDREAMBayesCalibration::calibrate().

The documentation for this class was generated from the following files:

- NonDDREAMBayesCalibration.hpp
- NonDDREAMBayesCalibration.cpp

13.100 NonDExpansion Class Reference

Base class for polynomial chaos expansions (PCE) and stochastic collocation (SC)

Inheritance diagram for NonDExpansion:

```
NonDExpansion
  |   NonDPolynomialChaos
  |   NonDStochCollocation
  
  NonD
  
  Analyzer
  
  Iterator
```
Public Member Functions

- **NonDExpansion** (ProblemDescDB &problem_db, Model &model)
  
  standard constructor

- **NonDExpansion** (unsigned short method_name, Model &model, short exp_coeffs_approach, short u_space_type, bool piecewise_basis, bool use_derivs)
  
  alternate constructor

- **~NonDExpansion** ()
  
  destructor

- **bool resize ()**
  
  reinitializes iterator based on new variable size

- **void derived_init_communicators** (ParLevLIter pl_iter)
  
  derived class contributions to initializing the communicators associated with this Iterator instance

- **void derived_set_communicators** (ParLevLIter pl_iter)
  
  derived class contributions to setting the communicators associated with this Iterator instance

- **void derived_free_communicators** (ParLevLIter pl_iter)
  
  derived class contributions to freeing the communicators associated with this Iterator instance

- **void core_run ()**
  
  perform a forward uncertainty propagation using PCE/SC methods

- **void print_results** (std::ostream &s)
  
  print the final statistics

- **const Model & algorithm_space_model () const**

- **virtual void select_refinement_points** (const RealVectorArray &candidate_samples, unsigned short batch_size, RealMatrix &best_samples)
  
  evaluate allSamples for inclusion in the (PCE regression) approximation and retain the best set (well spaced) of size batch_size

- **virtual void append_expansion** (const RealMatrix &samples, const IntResponseMap &resp_map)
  
  append new data to uSpaceModel and update expansion order (PCE only)

Protected Member Functions

- **virtual void resolve_inputs** (short &u_space_type, short &data_order)
  
  perform error checks and mode overrides

- **virtual void initialize_u_space_model ()**
  
  initialize uSpaceModel polynomial approximations with PCE/SC data

- **virtual void initialize_expansion ()**
  
  initialize random variable definitions and final stats arrays

- **virtual void compute_expansion ()**
  
  form the expansion by calling uSpaceModel.build_approximation()

- **virtual void increment_order_and_grid ()**
  
  uniformly increment the expansion order and structured/unstructured grid (PCE only)

- **virtual void increment_specification_sequence ()**
  
  increment the input specification sequence (PCE only)

- **virtual void update_expansion ()**
  
  update an expansion; avoids overhead in compute_expansion()
• virtual void multifidelity_expansion ()
  construct a multifidelity expansion, across model forms or discretization levels
• virtual void archive_coefficients ()
  archive expansion coefficients, as supported by derived instance
• virtual Real compute_covariance_metric ()
  compute 2-norm of change in response covariance
• virtual Real compute_final_statistics_metric ()
  compute 2-norm of change in final statistics
• void initialize_response_covariance ()
  set covarianceControl defaults and shape respCovariance
• void update_final_statistics ()
  update function values within finalStatistics
• void update_final_statistics_gradients ()
  update function gradients within finalStatistics
• void initialize (short u_space_type)
  common constructor code for initialization of natafTransform
• void check_dimension_preference (const RealVector &dim_pref) const
  check length and content of dimension preference vector
• void refine_expansion ()
  refine the reference expansion found by compute_expansion() using uniform/adaptive p-/h-refinement strategies
• void construct_cubature (Iterator &u_space_sampler, Model &g_u_model, unsigned short cub_int_order)
  assign a NonDCubature instance within u_space_sampler
• void construct_quadrature (Iterator &u_space_sampler, Model &g_u_model, const UShortArray &quad_order_seq, const RealVector &dim_pref)
  assign a NonDQuadrature instance within u_space_sampler based on a quad_order specification
• void construct_quadrature (Iterator &u_space_sampler, Model &g_u_model, int filtered_samples, const RealVector &dim_pref)
  assign a NonDQuadrature instance within u_space_sampler that generates a filtered tensor product sample set
• void construct_quadrature (Iterator &u_space_sampler, Model &g_u_model, int random_samples, int seed, const UShortArray &quad_order_seq, const RealVector &dim_pref)
  assign a NonDQuadrature instance within u_space_sampler that samples randomly from a tensor product multi-index
• void construct_sparse_grid (Iterator &u_space_sampler, Model &g_u_model, const UShortArray &ssg_level_seq, const RealVector &ssg_dim_pref)
  assign a NonDSparseGrid instance within u_space_sampler
• void construct_expansion_sampler (const String &import_approx_file, unsigned short import_approx_format=TABULAR_ANNOTATED, bool import_approx_active_only=false)
  construct the expansionSampler for evaluating samples on uSpaceModel
• void compute_statistics ()
  calculate analytic and numerical statistics from the expansion
• void archive_moments ()
  archive the central moments (numerical and expansion) to ResultsDB
Protected Attributes

- **Model uSpaceModel**
  - *Model* representing the approximate response function in u-space, after u-space recasting and polynomial data fit recursions.
- **short expansionCoeffsApproach**
  - method for collocation point generation and subsequent calculation of the expansion coefficients
- **short expansionBasisType**
  - type of expansion basis: DEFAULT BASIS or Pecos::{NODAL,HIERARCHICAL}_INTERPOLANT for SC or Pecos::{TENSOR_PRODUCT,TOTAL_ORDER,ADAPTED}_BASIS for PCE regression
- **size_t numUncertainQuant**
  - number of invocations of core_run()
- **int numSamplesOnModel**
  - number of truth samples performed on g_u_model to form the expansion
- **int numSamplesOnExpansion**
  - number of approximation samples performed on the polynomial expansion in order to estimate probabilities
- **bool nestedRules**
  - flag for indicating state of nested and non_nested overrides of default rule nesting, which depends on the type of integration driver
- **bool piecewiseBasis**
  - flag for piecewise specification, indicating usage of local basis polynomials within the stochastic expansion
- **bool useDerivs**
  - flag for use_derivatives specification, indicating usage of derivative data (with respect to expansion variables) to enhance the calculation of the stochastic expansion.
- **short refineType**
  - refinement type: NO_REFINEMENT, P_REFINEMENT, or H_REFINEMENT
- **short refineControl**
  - refinement control: NO_CONTROL, UNIFORM_CONTROL, LOCAL_ADAPTIVE_CONTROL, DIMENSION_ADAPTIVE_CONTROL_SOBO, DIMENSION_ADAPTIVE_CONTROL_DECAY, or DIMENSION_ADAPTIVE_CONTROL_GENERALIZED
- **unsigned short softConvLimit**
  - number of consecutive iterations within tolerance required to indicate soft convergence
- **RealSymMatrix respCovariance**
  - symmetric matrix of analytic response covariance (full response covariance option)
- **RealVector respVariance**
  - vector of response variances (diagonal response covariance option)
- **RealVector initialPtU**
  - stores the initial variables data in u-space

Private Member Functions

- **void reduce_total_sobol_sets** (RealVector &avg_sobol)
  - compute average of total Sobol’ indices (from VBD) across the response set for use as an anisotropy indicator
- **void reduce_decay_rate_sets** (RealVector &min_decay)
  - compute minimum of spectral coefficient decay rates across the response set for use as an anisotropy indicator
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- **void initialize_sets ()**
  
  Initialization of adaptive refinement using generalized sparse grids

- **Real increment_sets ()**
  
  Perform an adaptive refinement increment using generalized sparse grids

- **void finalize_sets (bool converged, within, tol)**
  
  Finalization of adaptive refinement using generalized sparse grids

- **void compute_analytic_statistics ()**
  
  Analytic portion of compute_statistics() from post-processing of expansion coefficients

- **void compute_numerical_statistics ()**
  
  Numerical portion of compute_statistics() from sampling on the expansion

- **void compute_numerical_stat_refinements (RealVectorArray &imp_sampler_stats, RealRealPairArray &min_max_fns)**
  
  Refinements to numerical probability statistics from importanceSampler

- **void compute_covariance ()**
  
  Calculate the response covariance (diagonal or full matrix)

- **void compute_diagonal_variance ()**
  
  Calculate respVariance or diagonal terms respCovariance(i,i)

- **void compute_off_diagonal_covariance ()**
  
  Calculate respCovariance(i,j) for j<i

- **void print_moments (std::ostream &s)**
  
  Print expansion and numerical moments

- **void print_covariance (std::ostream &s)**
  
  Print respCovariance

- **void print_sobol_indices (std::ostream &s)**
  
  Print global sensitivity indices

- **void print_local_sensitivity (std::ostream &s)**
  
  Print local sensitivities evaluated at initialPtU

- **void compute_print_increment_results ()**
  
  Manage print of results following a refinement increment

- **void compute_print_iteration_results (bool initialize)**
  
  Manage print of results following a refinement increment

- **void compute_print_converged_results (bool print_override=false)**
  
  Manage print of results following convergence of iterative refinement

**Private Attributes**

- **short ruleNestingOverride**
  
  User override of default rule nesting: NO_NESTING_OVERRIDE, NESTED, or NON_NESTED

- **short ruleGrowthOverride**
  
  User override of default rule growth: NO_GROWTH_OVERRIDE, RESTRICTED, or UNRESTRICTED

- **Iterator expansionSampler**
  
  Iterator used for sampling on the uSpaceModel to generate approximate probability/reliability/response level statistics. Currently this is an LHS sampling instance, but AIS could also be used.

- **Iterator importanceSampler**
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Iterate used to refine the approximate probability estimates generated by the expansionSampler using importance sampling.

• RealMatrix expGradsMeanX
derivative of the expansion with respect to the x-space variables evaluated at the means (used as uncertainty importance metrics)

• int maxRefineIterations
maximum number of uniform/adaptive refinement iterations (specialization of maxIterations)

• int maxSolverIterations
maximum number of regression solver iterations (specialization of maxIterations)

• bool vbdFlag
flag indicating the activation of variance-based decomposition for computing Sobol' indices

• unsigned short vbdOrderLimit
limits the order of interactions within the component Sobol' indices

• Real vbdDropTol
tolerance for omitting output of small VBD indices

• short covarianceControl
enumeration for controlling response covariance calculation and output: {DEFAULT,DIAGONAL,FULL}.COVARIANCE

• unsigned short integrationRefine
integration refinement for expansion sampler

• String expansionRng
random number generator for expansion sampler

• int origSeed
seed for expansion sampler random number generator

• unsigned short expansionSampleType
sample type for expansion sampler

• IntVector refinementSamples
refinement samples for expansion sampler

Additional Inherited Members

13.100.1 Detailed Description

Base class for polynomial chaos expansions (PCE) and stochastic collocation (SC)

The NonDExpansion class provides a base class for methods that use polynomial expansions to approximate the effect of parameter uncertainties on response functions of interest.

13.100.2 Member Function Documentation

const Model & algorithm_space_model() const [inline], [virtual]
default definition that gets redefined in selected derived Minimizers

Reimplemented from Analyzer.
References NonDExpansion::uSpaceModel.
void increment_specification_sequence( ) [protected], [virtual]

increment the input specification sequence (PCE only)
  default implementation is overridden by PCE
  Reimplemented in NonDPolynomialChaos.
  References NonDIntegration::increment_specification_sequence(), Iterator::iterator_rep(), Model::subordinate_iterator(), and NonDExpansion::uSpaceModel.
  Referenced by NonDPolynomialChaos::increment_specification_sequence(), and NonDExpansion::multifidelity_expansion().

Real compute_covariance_metric( ) [protected], [virtual]

compute 2-norm of change in response covariance
  computes the default refinement metric based on change in respCovariance
  Reimplemented in NonDStochCollocation.
  References NonDExpansion::compute_covariance(), NonDExpansion::covarianceControl, NonDExpansion::respCovariance, and NonDExpansion::respVariance.
  Referenced by NonDStochCollocation::compute_covariance_metric(), NonDExpansion::increment_sets(), and NonDExpansion::refine_expansion().

Real compute_final_statistics_metric( ) [protected], [virtual]

compute 2-norm of change in final statistics
  computes a "goal-oriented" refinement metric employing finalStatistics
  Reimplemented in NonDStochCollocation.
  References NonDExpansion::compute_statistics(), NonD::finalMomentsType, NonD::finalStatistics, Response::function_values(), Analyzer::numFunctions, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, and NonD::requestedRespLevels.
  Referenced by NonDStochCollocation::compute_final_statistics_metric(), and NonDExpansion::increment_sets().

void compute_statistics( ) [protected]

calculate analytic and numerical statistics from the expansion
  Calculate analytic and numerical statistics from the expansion and log results within final_stats for use in OUU.
  References ResultsManager::active(), NonDExpansion::archive_coefficients(), NonDExpansion::archive_moments(), NonDExpansion::compute_analytic_statistics(), NonDExpansion::compute_numerical_statistics(), Model::continuous_variable_labels(), Model::continuous_variables(), NonDExpansion::expansionSampler, NonDExpansion::expGradsMeanX, NonD::initialize_level_mappings(), NonDExpansion::initialPtU, ResultsManager::insert(), Iterator::is_null(), Iterator::iteratedModel, Analyzer::numContinuousVars, Analyzer::numFunctions, Iterator::outputLevel, Model::response_labels(), Iterator::resultsDB, Iterator::resultsNames, Iterator::run_identifier(), Iterator::subIterFlag, NonD::totalLevelRequests, and NonDExpansion::uSpaceModel.
  Referenced by NonDStochCollocation::compute_final_statistics_metric(), NonDExpansion::compute_final_statistics_metric(), NonDExpansion::compute_print_converged_results(), NonDExpansion::compute_print_increment_results(), and NonDExpansion::compute_print_iteration_results().
13.100.3 Member Data Documentation

`bool useDerivs [protected]`

flag for `use_derivatives` specification, indicating usage of derivative data (with respect to expansion variables) to enhance the calculation of the stochastic expansion.

This is part of the method specification since the instantiation of the global data fit surrogate is implicit with no user specification. This behavior is distinct from the usage of response derivatives with respect to auxiliary variables (design, epistemic) for computing derivatives of aleatory expansion statistics with respect to these variables.

Referenced by NonDExpansion::compute_expansion(), NonDStochCollocation::initialize_u_space_model(), NonDPolynomialChaos::initialize_u_space_model(), NonDPolynomialChaos::ratio_samples_to_order(), NonDStochCollocation::resolve_inputs(), NonDPolynomialChaos::resolve_inputs(), NonDPolynomialChaos::terms_ratio_to_samples(), and NonDPolynomialChaos::terms_samples_to_ratio().

The documentation for this class was generated from the following files:

- NonDExpansion.hpp
- NonDExpansion.cpp

13.101 NonDGlobalEvidence Class Reference

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

Inheritance diagram for NonDGlobalEvidence:

```
   NonDGlobalEvidence
    └── NonDInterval
        └── NonD
            └── NonDAnalyzer
                └── Iterator
```

Public Member Functions

- `NonDGlobalEvidence (ProblemDescDB &problem_db, Model &model)`
  constructor
- `~NonDGlobalEvidence ()`
  destructor
- `void initialize ()`
  perform any required initialization
- `void set_cell_bounds ()`
Additional Inherited Members

13.101.1 Detailed Description

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

The NonDEvidence class implements the propagation of epistemic uncertainty using Dempster-Shafer theory of evidence. In this approach, one assigns a set of basic probability assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated, along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response surface is constructed which is sampled extensively to find the minimum and maximum within each input interval cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to calculate cumulative distribution functions for belief and plausibility.

The documentation for this class was generated from the following files:

- NonDGlobalEvidence.hpp
- NonDGlobalEvidence.cpp

13.102 NonDGlobalInterval Class Reference

Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDGlobalInterval:
Public Member Functions

- **NonDGlobalInterval** (ProblemDescDB &problem_db, Model &model)
  
  constructor

- **~NonDGlobalInterval** ()
  
  destructor

- **void derived_init_communicators** (ParLevLIter pl_iter)
  
  derived class contributions to initializing the communicators associated with this Iterator instance

- **void derived_set_communicators** (ParLevLIter pl_iter)
  
  derived class contributions to setting the communicators associated with this Iterator instance

- **void derived_free_communicators** (ParLevLIter pl_iter)
  
  derived class contributions to freeing the communicators associated with this Iterator instance

- **void core_run** ()
  
  Performs an optimization to determine interval bounds for an entire function or interval bounds on a particular statistical estimator.

- **const Model & algorithm_space_model** () const

Protected Member Functions

- **virtual void initialize** ()
  
  perform any required initialization

- **virtual void set_cell_bounds** ()
  
  set the optimization variable bounds for each cell

- **virtual void get_best_sample** (bool maximize, bool eval_approx)
  
  determine truthFnsStar and approxFnsStar

- **virtual void post_process_cell_results** (bool maximize)
  
  post-process a cell minimization/maximization result

- **virtual void post_process_response_fn_results** ()
  
  post-process the interval computed for a response function

- **virtual void post_process_final_results** ()
  
  perform final post-processing

- **void post_process_run_results** (bool maximize)
  
  post-process an optimization execution: output results, update convergence controls, and update GP approximation

- **void evaluate_response_star_truth** ()
  
  evaluate the truth response at the optimal variables solution and update the GP with the new data

Protected Attributes

- **Iterator daceIterator**
  
  LHS iterator for constructing initial GP for all response functions.

- **Model fHatModel**
  
  GP model of response, one approximation per response function.

- **Iterator intervalOptimizer**
  
  optimizer for solving surrogate-based subproblem: NCSU DIRECT optimizer for maximizing expected improvement or mixed EA if discrete variables.
• Model intervalOptModel
  recast model which formulates the surrogate-based optimization subproblem (recasts as design problem; may assimilate mean and variance to enable max(expected improvement))

• Real approxFnStar
  approximate response corresponding to minimum/maximum truth response

• Real truthFnStar
  minimum/maximum truth response function value

Static Private Member Functions

• static void EIF_objective_min (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  static function used as the objective function in the Expected Improvement Function (EIF) for minimizing the GP

• static void EIF_objective_max (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  static function used as the objective function in the Expected Improvement Function (EIF) for maximizing the GP

• static void extract_objective (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  static function used to extract the active objective function when optimizing for an interval lower or upper bound (non-EIF formulations). The sense of the optimization is set separately.

Private Attributes

• const int seedSpec
  the user seed specification (default is 0)

• int numSamples
  the number of samples used in the surrogate

• String rngName
  name of the random number generator

• bool gpModelFlag
  flag indicating use of GP surrogate emulation

• bool eifFlag
  flag indicating use of maximized expected improvement for GP iterate selection

• unsigned short improvementConvergeCntr
  counter for number of successive iterations that the iteration improvement is less than the convergenceTol

• unsigned short improvementConvergeLimit
  counter for number of successive iterations that the iteration improvement is less than the convergenceTol

• Real distanceTol
  tolerance for \(L_2\) change in optimal solution

• unsigned short distanceConvergeCntr
  counter for number of successive iterations that the \(L_2\) change in optimal solution is less than the convergenceTol

• unsigned short distanceConvergeLimit
  counter for number of successive iterations that the \(L_2\) change in optimal solution is less than the convergenceTol

• RealVector prevCVStar
  stores previous optimal point for continuous variables; used for assessing convergence
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- IntVector prevDIVStar
  stores previous optimal point for discrete integer variables; used for assessing convergence
- RealVector prevDRVStar
  stores previous optimal point for discrete real variables; used for assessing convergence
- Real prevFnStar
  stores previous solution value for assessing convergence
- size_t globalIterCntr
  global iteration counter for number of surrogate-based min/max solves
- bool boundConverged
  flag indicating convergence of a minimization or maximization cycle
- bool allResponsesPerIter
  flag for maximal response extraction (all response values obtained on each function call)
- short dataOrder
  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format; user may override

Static Private Attributes
- static NonDGlobalInterval * nondGIInstance
  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

13.102.1 Detailed Description

Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

The NonDGlobalInterval class supports global nongradient-based optimization approaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval analysis (e.g. intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels. The preliminary implementation will use a Gaussian process surrogate to determine interval bounds.

13.102.2 Member Function Documentation

const Model & algorithm_space_model ( ) const [inline], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Analyzer.
References NonDGlobalInterval::fHatModel.
The documentation for this class was generated from the following files:

- NonDGlobalInterval.hpp
- NonDGlobalInterval.cpp
13.103 NonDGlobalReliability Class Reference

Class for global reliability methods within DAKOTA/UQ.

Inheritance diagram for NonDGlobalReliability:

```
  NonDGlobalReliability
  |                   |
  |                   |
  V                   V
  NonDReliability
  |                   |
  |                   |
  V                   V
  NonD
  |                   |
  |                   |
  V                   V
  Analyzer
  |                   |
  |                   |
  V                   V
  Iterator
```

Public Member Functions

- **NonDGlobalReliability** (ProblemDescDB &problem_db, Model &model)
  constructor

- ~NonDGlobalReliability ()
  destructor

- **bool resize ()**
  reinitializes iterator based on new variable size

- **void derived_init_communicators** (ParLevLIter pl_iter)
  derived class contributions to initializing the communicators associated with this Iterator instance

- **void derived_set_communicators** (ParLevLIter pl_iter)
  derived class contributions to setting the communicators associated with this Iterator instance

- **void derived_free_communicators** (ParLevLIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance

- **void core_run ()**
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

- **void print_results** (std::ostream &s)
  print the final iterator results

Private Member Functions

- **void optimize_gaussian_process ()**
  construct the GP using EGO/SKO

- **void importance_sampling ()**
  perform multimodal adaptive importance sampling on the GP

- **void get_best_sample ()**
  determine current best solution from among sample data for expected improvement function in Performance Measure Approach (PMA)
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- **Real** `constraint_penalty (const Real &constraint, const RealVector &c_variables)`
  calculate the penalty to be applied to the PMA constraint value
- **Real** `expected_improvement (const RealVector &expected_values, const Variables &recast_vars)`
  expected improvement function for the GP
- **Real** `expected_feasibility (const RealVector &expected_values, const Variables &recast_vars)`
  expected feasibility function for the GP

**Static Private Member Functions**

- **static void** `EIF_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)`
  static function used as the objective function in the Expected Improvement (EIF) problem formulation for PMA
- **static void** `EFF_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)`
  static function used as the objective function in the Expected Feasibility (EFF) problem formulation for RIA

**Private Attributes**

- **Real** `fnStar`
  minimum penalized response from among true function evaluations
- **short** `meritFunctionType`
  type of merit function used to penalize sample data
- **Real** `lagrangeMult`
  Lagrange multiplier for standard Lagrangian merit function.
- **Real** `augLagrangeMult`
  Lagrange multiplier for augmented Lagrangian merit function.
- **Real** `penaltyParameter`
  penalty parameter for augmented Lagrangian merit function.
- **Real** `lastConstraintViolation`
  constraint violation at last iteration, used to determine if the current iterate should be accepted (must reduce violation)
- **bool** `lastIterateAccepted`
  flag to determine if last iterate was accepted this controls update of parameters for augmented Lagrangian merit function
- **short** `dataOrder`
  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format; user may override responses spec

**Static Private Attributes**

- **static NonDGlobalReliability** `∗nondGlobRelInstance`
  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data
13.103.1 Detailed Description

Class for global reliability methods within DAKOTA/UQ.

The NonDGlobalReliability class implements EGO/SKO for global MPP search, which maximizes an expected improvement function derived from Gaussian process models. Once the limit state has been characterized, a multimodal importance sampling approach is used to compute probabilities.

13.103.2 Member Function Documentation

void core_run( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References NonDGlobalReliability::importance_sampling(), NonD::initialize_random_variable_parameters(), NonDGlobalReliability::nondGlobRelInstance, NonDReliability::numRelAnalyses, NonDGlobalReliability::optimize_gaussian_process(), and NonD::transform_correlations().

void print_results ( std::ostream & s ) [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References NonD::cdfFlag, NonD::computedGenRelLevels, NonD::computedProbLevels, NonD::computed-RespLevels, Iterator::iteratedModel, Analyzer::numFunctions, NonD::print_densities(), Model::response_labels(), and Dakota::write_precision.

The documentation for this class was generated from the following files:

- NonDGlobalReliability.hpp
- NonDGlobalReliability.cpp

13.104 NonDGlobalSingleInterval Class Reference

Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDGlobalSingleInterval:
The NonDGlobalSingleInterval class supports global nongradient-based optimization approaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval analysis (e.g. intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels. The preliminary implementation will use a Gaussian process surrogate to determine interval bounds.

The documentation for this class was generated from the following files:
13.105 NonDGPImpSampling Class Reference

Class for the Gaussian Process-based Importance Sampling method.

Inheritance diagram for NonDGPImpSampling:

```
NonDGPImpSampling
  NonDSampling
    NonD
      Analyzer
        Iterator
```

Public Member Functions

- **NonDGPImpSampling (ProblemDescDB &problem_db, Model &model)**
  
  *standard constructor*

- **~NonDGPImpSampling ()**

  *destructor*

- **bool resize ()**

  *reinitializes iterator based on new variable size*

- **void derived_init_communicators (ParLevLIter pl_iter)**

  *derived class contributions to initializing the communicators associated with this Iterator instance*

- **void derived_set_communicators (ParLevLIter pl_iter)**

  *derived class contributions to setting the communicators associated with this Iterator instance*

- **void derived_free_communicators (ParLevLIter pl_iter)**

  *derived class contributions to freeing the communicators associated with this Iterator instance*

- **void core_run ()**

  *perform the GP importance sampling and return probability of failure*

- **void print_results (std::ostream &s)**

  *print the final statistics*

- **Real final_probability ()**

  *returns the probability calculated by the importance sampling*
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Private Member Functions

- RealVector calcExpIndicator (const int respFnCount, const Real respThresh)
  
  *function to calculate the expected indicator probabilities*

- Real calcExpIndPoint (const int respFnCount, const Real respThresh, const RealVector this_mean, const RealVector this_var)
  
  *function to calculate the expected indicator probabilities for one point*

- void calcRhoDraw ()
  
  *function to update the rhoDraw data, adding x values and rho draw values*

- RealVector drawNewX (int this_k)
  
  *function to pick the next X value to be evaluated by the Iterated model*

Private Attributes

- Iterator gpBuild
  
  *LHS iterator for building the initial GP.*

- Iterator gpEval
  
  *LHS iterator for sampling on the GP.*

- Model gpModel
  
  *GP model of response, one approximation per response function.*

- Iterator sampleRhoOne
  
  *LHS iterator for sampling from the rhoOneDistribution.*

- int numPtsAdd
  
  *the number of points added to the original set of LHS samples*

- int numPtsTotal
  
  *the total number of points*

- int numEmulEval
  
  *the number of points evaluated by the GP each iteration*

- Real finalProb
  
  *the final calculated probability (p)*

- RealVectorArray gpCvars
  
  *Vector to hold the current values of the current sample inputs on the GP.*

- RealVectorArray gpMeans
  
  *Vector to hold the current values of the current mean estimates for the sample values on the GP.*

- RealVectorArray gpVar
  
  *Vector to hold the current values of the current variance estimates for the sample values on the GP.*

- RealVector expIndicator
  
  *Vector to hold the expected indicator values for the current GP samples.*

- RealVector rhoDraw
  
  *Vector to hold the rhoDraw values for the current GP samples.*

- RealVector normConst
  
  *Vector to hold the normalization constant calculated for each point added.*

- RealVector indicator
  
  *IntVector to hold indicator for actual simulation values vs. threshold.*
• RealVectorArray \( xDrawThis \)
  \( xDrawThis \), appended locally to hold the X values of emulator points chosen

• RealVector \( \text{expIndThis} \)
  \( \text{expIndThis} \), appended locally to hold the expected indicator

• RealVector \( \text{rhoDrawThis} \)
  \( \text{rhoDrawThis} \), appended locally to hold the \( \text{rhoDraw} \) density for calculating draws

• RealVector \( \text{rhoMix} \)
  \( \text{rhoMix} \), mixture density

• RealVector \( \text{rhoOne} \)
  \( \text{rhoOne} \), original importance density

Additional Inherited Members

13.105.1 Detailed Description

Class for the Gaussian Process-based Importance Sampling method.

The \text{NonDGPImpSampling} implements a method developed by Keith Dalbey that uses a Gaussian process surrogate in the calculation of the importance density. Specifically, the mean and variance of the GP prediction are used to calculate an expected value that a particular point fails, and that is used as part of the computation of the "draw distribution." The normalization constants and the mixture distribution used are defined in (need to get SAND report).

13.105.2 Constructor & Destructor Documentation

\text{NonDGPImpSampling} ( \text{ProblemDescDB} & \text{problem\_db}, \text{Model} & \text{model} )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db\_list\_nodes has been called and probDescDB can be queried for settings from the method specification.

References Response::active\_set(), Iterator::assign\_rep(), Model::assign\_rep(), NonD::construct\_lhs(), Model::current\_response(), ProblemDescDB::get\_bool(), ProblemDescDB::get\_int(), ProblemDescDB::get\_string(), ProblemDescDB::get\_ushort(), NonDGPImpSampling::gpBuild, NonDGPImpSampling::gpEval, NonDGPImpSampling::gpModel, Model::gradient\_type(), Model::hessian\_type(), Iterator::iteratedModel, Iterator::max\_Iterations, NonDGPImpSampling::num\_Emul\_Eval, NonDGPImpSampling::num\_Pts\_Add, NonDSampling::num\_Samples, Iterator::output\_Level, Iterator::probDescDB, NonDSampling::random\_Seed, ActiveSet::request\_values(), NonDSampling::rng\_Name, NonDGPImpSampling::sample\_Rho\_One, NonDSampling::sample\_Type, NonDSampling::sampling\_Vars\_Mode, NonDSampling::stats\_Flag, NonDSampling::vary\_pattern(), and NonDSampling::vary\_Pattern.

13.105.3 Member Function Documentation

\text{void core\_run() \ [virtual]}

perform the GP importance sampling and return probability of failure

Calculate the failure probabilities for specified probability levels using Gaussian process based importance sampling.

Reimplemented from \text{Iterator}.

References Model::acv(), Iterator::all\_responses(), Analyzer::all\_samples(), Iterator::all\_samples(), Model::append\_approximation(), Model::approximation\_data(), Model::approximation\_variances(), Model::build\_approximation(),

...
NonDGPImpSampling::calcExpIndicator(), NonDGPImpSampling::calcExpIndPoint(), NonDGPImpSampling::calcRhoDraw(), NonD::cdfFlag, NonD::computedProbLevels, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Model::current_response(), Model::current_variables(), NonDGPImpSampling::drawNewX(), Model::evaluate(), Model::evaluation_id(), NonDGPImpSampling::expIndicator, NonDGPImpSampling::expIndThis, NonDGPImpSampling::finalProb, Response::function_values(), NonDGPImpSampling::gpCvars, NonDGPImpSampling::gpEval, NonDGPImpSampling::gpMeans, NonDGPImpSampling::gpModel, NonDGPImpSampling::gpVar, NonDGPImpSampling::indicatore, NonD::initialize_level_mappings(), Iterator::iteratedModel, Iterator::methodPCIter, NonD::miPLIndex, NonDGPImpSampling::normConst, NonDGPImpSampling::numEmulEval, Analyzer::numFunctions, NonDGPImpSampling::numPtsAdd, NonDGPImpSampling::numPtsTotal, NonDSampling::numSamples, Iterator::outputLevel, Model::pop_approximation(), NonD::requestedRespLevels, NonDGPImpSampling::rhoDraw, NonDGPImpSampling::rhoDrawThis, NonDGPImpSampling::rhoMix, NonDGPImpSampling::rhoOne, Iterator::run(), NonDGPImpSampling::sampleRhoOne, and NonDGPImpSampling::xDrawThis.

The documentation for this class was generated from the following files:

- NonDGPImpSampling.hpp
- NonDGPImpSampling.cpp

### 13.106 NonDGPMsABayesCalibration Class Reference

Generates posterior distribution on model parameters given experiment data.

Inheritance diagram for NonDGPMsABayesCalibration:

```
  Iterator
  |   
  v
Analyzer
  |   
  v
NonD
  |   
  v
NonDCalibration
  |   
  v
NonDBayesCalibration
  |   
  v
NonDQUESOBayesCalibration
  |   
  v
NonDGPMsABayesCalibration
```

#### Public Member Functions

- **NonDGPMsABayesCalibration** (ProblemDescDB &problem_db, Model &model)
  
  *constructor*

- **~NonDGPMsABayesCalibration** ()
  
  *destructor*
Protected Member Functions

- void derived_init_communicators (ParLevIter pl_iter)
  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevIter pl_iter)
  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance
- void calibrate ()
  performs a forward uncertainty propagation by using GPM/SA to generate a posterior distribution on parameters
  given a set of simulation parameter/response data, a set of experimental data, and additional variables to be
  specified here.
- void init_queso_solver ()
  specialization to initialize the inverse problem and posterior
- void acquire_simulation_data ()
  Populate simulation data (run design of experiments or load build data)
- void normalize_configs ()
  Determine each scenario min/max and set GPMSA scaling options.
- void overlay_proposal_covariance (QUESO::GslMatrix &full_prop_cov) const
  fill the full proposal covariance, including hyperparameter entries with user-specified or default theta covariance
  information
- void fill_simulation_data (bool scale_data)
  populate the simulation data, calculating and applying scaling if needed
- void fill_experiment_data (bool scale_data)
  populate the experiment data, applying scaling if needed
- void overlay_initial_params (QUESO::GslVector &full_param_initials)
  overlay the Dakota user's initial parameters on the full GPMSA vector of parameters
- void cache_acceptance_chain ()
  retrieve the chain from QUESO and populate acceptanceChain / acceptedFnVals
- void print_results (std::ostream &s)
  print the final iterator results

Protected Attributes

- int buildSamples
  number of samples of the simulation to construct the GP
- String approxImportFile
  name of file from which to import build points to build GP
- unsigned short approxImportFormat
  build data import tabular format
- bool approxImportActiveOnly
  import active variables only
- unsigned int userConfigVars
  number of user-specified configuration (scenario) vars
- unsigned int gpmsaConfigVars
number of config vars presented to GPMSA (minimum 1)

• bool gpmsaNormalize
  whether to apply GPMSA-internal variable and data normalization

• boost::shared_ptr
  < QUESO::VectorSpace
  < QUESO::GslVector,
  QUESO::GslMatrix >> configSpace
  vector space defining the scenario (configuration) variables

• boost::shared_ptr
  < QUESO::VectorSpace
  < QUESO::GslVector,
  QUESO::GslMatrix >> nEtaSpace
  vector space defining the output (response) space for the simulations

• boost::shared_ptr
  < QUESO::VectorSpace
  < QUESO::GslVector,
  QUESO::GslMatrix >> experimentSpace
  vector space defining the output (response) space for the experiments

• RealMatrix simulationData
  simulation data, one row per simulation build sample, columns for calibration variables, configuration variables, function values (duplicates storage, but unifies import vs. DOE cases)

• RealVector simulationMean
  simulation mean values for scaling, one per function

• RealVector simulationStdDev
  simulation std deviations for scaling, one per function

• boost::shared_ptr
  < QUESO::GPMSAOptions > gpmsaOptions
  Configuration options for the GPMSA solver.

• String optionsFile
  advanced options file name

• boost::shared_ptr
  < QUESO::GPMSAFactory
  < QUESO::GslVector,
  QUESO::GslMatrix >> gpmsaFactory
  core factory that manages a GP-based likelihood

Private Attributes

• Iterator lhsIter
  LHS iterator for generating samples for GP.

Static Private Attributes

• static NonDGPSABayesCalibration * nonDGPMSAInstance
  Pointer to current class instance for use in static callback functions.
Additional Inherited Members

13.106.1 Detailed Description

Generates posterior distribution on model parameters given experiment data.

This class provides a wrapper for the functionality provided in the Los Alamos National Laboratory code called GPM/SA (Gaussian Process Models for Simulation Analysis). Although this is a code that provides input/output mapping, it DOES NOT provide the mapping that we usually think of in the NonDeterministic class hierarchy in DAKOTA, where uncertainty in parameter inputs are mapped to uncertainty in simulation responses. Instead, this class takes a pre-existing set of simulation data as well as experimental data, and maps priors on input parameters to posterior distributions on those input parameters, according to a likelihood function. The goal of the MCMC sampling is to produce posterior values of parameter estimates which will produce simulation response values that "match well" to the experimental data. The MCMC is an integral part of the calibration. The data structures in GPM/SA are fairly detailed and nested. Part of this prototyping exercise is to determine what data structures need to be specified and initialized in DAKOTA and sent to GPM/SA, and what data structures will be returned.

13.106.2 Constructor & Destructor Documentation

NonDGPMsABayesCalibration ( ProblemDescDB & problem_db, Model & model )

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDGPMsABayesCalibration::approxImportActiveOnly, NonDGPMsABayesCalibration::approxImportFile, Iterator::assign(), NonDGPMsABayesCalibration::buildSamples, Model::current_response(), NonDBayesCalibration::emulatorType, NonDCalibration::expData, ProblemDescDB::get_string(), NonDQUESOBayesCalibration::init_queso_environment(), NonDGPMsABayesCalibration::hsIter, NonDBayesCalibration::mcmcModel, ExperimentData::num_experiments(), SharedResponseData::num_field_response_groups(), NonDGPMsABayesCalibration::optionsFile, Iterator::outputLevel, Iterator::probDescDB, NonDBayesCalibration::randomSeed, Response::shared_data(), and NonDGPMsABayesCalibration::userConfigVars.

13.106.3 Member Function Documentation

void calibrate ( ) [protected], [virtual]

performs a forward uncertainty propagation by using GPM/SA to generate a posterior distribution on parameters given a set of simulation parameter/response data, a set of experimental data, and additional variables to be specified here.

Perform the uncertainty quantification

Implements NonDBayesCalibration.

References NonDGPMsABayesCalibration::acquire_simulation_data(), ExperimentData::all_data(), NonDGPMsABayesCalibration::buildSamples, NonDGPMsABayesCalibration::cache_acceptance_chain(), NonDQUESOBayesCalibration::callMhOptionsValues, NonDBayesCalibration::compute_statistics(), NonDGPMsABayesCalibration::configSpace, NonDCalibration::expData, NonDGPMsABayesCalibration::experimentSpace, NonDGPMsABayesCalibration::fill_experiment_data(), NonDGPMsABayesCalibration::fill_simulation_data(), NonDGPMsABayesCalibration::gpmseFactory, NonDGPMsABayesCalibration::gpmseNormalize, NonDGPMsABayesCalibration::gpmseOptions, NonDQUESOBayesCalibration::init_parameter_domain(), NonDGPMsABayesCalibration::init_queso_solver(), NonDBayesCalibration::initialize_model(), NonDQUESOBayesCalibration::mcmcType, NonDGPMsABayesCalibration::nEtaSpace, NonDGPMsABayesCalibration::nonDGPMsABayesInstance, NonDQUESOBayesCalibration::nonDQUESOInstance, NonDGPM-
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void normalize_configs() [protected]

Determine each scenario min/max and set GPMSA scaling options.

Check for valid vs. degenerate configuration variable scaling cases. If all configs for a variable are identical, scale them all to 0.5. Could also consider scaling them based on continuous state bounds if present...

References NonDGPMSABayesCalibration::buildSamples, NonDGPMSABayesCalibration::gpmsaOptions, Analyzer::numContinuousVars, Iterator::outputLevel, NonDGPMSABayesCalibration::simulationData, and NonDGPMSABayesCalibration::userConfigVars.

Referenced by NonDGPMSABayesCalibration::calibrate().

void cache_acceptance_chain() [protected]

retrieve the chain from QUESO and populate acceptanceChain / acceptedFnVals

This is a subset of the base class retrieval, but we can’t do the fn value lookups. Eventually should be able to retrieve them from GPMSA.

References NonDBayesCalibration::acceptanceChain, NonDBayesCalibration::acceptedFnVals, NonDBayesCalibration::chainCycles, NonDBayesCalibration::chainSamples, NonDQUESOBayesCalibration::copy_gsl_partial(), NonD::natafTransform, Analyzer::numContinuousVars, Analyzer::numFunctions, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, and NonDBayesCalibration::standardizedSpace.

Referenced by NonDGPMSABayesCalibration::calibrate().

void print_results(std::ostream & s) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from NonDBayesCalibration.

References NonDBayesCalibration::print_results().

The documentation for this class was generated from the following files:

- NonDGPMSABayesCalibration.hpp
- NonDGPMSABayesCalibration.cpp

13.107 NonDIntegration Class Reference

Derived nondeterministic class that generates N-dimensional numerical integration points for evaluation of expectation integrals.

Inheritance diagram for NonDIntegration:
Public Member Functions

- virtual void initialize_grid (const std::vector<Pecos::BasisPolynomial> &poly_basis)=0
  initialize integration grid by drawing from polynomial basis settings
- virtual void increment_grid ()=0
  increment SSG level/TPQ order
- virtual void increment_grid_preference (const RealVector &dim_pref)
  increment SSG level/TPQ order and update anisotropy
- virtual void increment_grid_weights (const RealVector &aniso_wts)
  increment SSG level/TPQ order and update anisotropy
- virtual void increment_specification_sequence ()
  increment sequenceIndex and update active orders/levels
- const Pecos::IntegrationDriver & driver () const
  return numIntDriver
- bool resize ()
  reinitializes iterator based on new variable size

Static Public Member Functions

- static void dimension_preference_to_anisotropic_order (unsigned short scalar_order_spec, const RealVector &dim_pref_spec, size_t num_v, UShortArray &aniso_order)
  convert scalar_order_spec and vector dim_pref_spec to vector aniso_order
- static void anisotropic_order_to_dimension_preference (const UShortArray &aniso_order, unsigned short &scalar_order, RealVector &dim_pref)
  convert vector aniso_order to scalar_order and vector dim_pref

Protected Member Functions

- NonDIntegration (ProblemDescDB &problem_db, Model &model)
  constructor
- NonDIntegration (unsigned short method_name, Model &model)
  alternate constructor for instantiations "on the fly"
• NonDIntegration (unsigned short method_name, Model &model, const RealVector &dim_pref)
  alternate constructor for instantiations "on the fly"
• ~NonDIntegration ()
  destructor
• void core_run ()
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
• void check_variables (const std::vector<Pecos::RandomVariable> &x_ran_vars)
  verify self-consistency of variables data
• void print_points_weights (const String &tabular_name)
  output integration points and weights to a tabular file

Protected Attributes

• Pecos::IntegrationDriver numIntDriver
  Pecos utility class for managing interface to tensor-product grids and VPISparseGrid utilities for Smolyak sparse
  grids and cubature.
• size_t numIntegrations
  counter for number of integration executions for this object
• size_t sequenceIndex
  index into NonDQuadrature::quadOrderSpec and NonDSparseGrid::ssgLevelSpec that defines the current instance
  of several possible refinement levels
• RealVector dimPrefSpec
  the user specification for anisotropic dimension preference

Additional Inherited Members

13.107.1 Detailed Description

Derived nondeterministic class that generates N-dimensional numerical integration points for evaluation of ex-
pectation integrals.

This class provides a base class for shared code among NonDQuadrature and NonDSparseGrid.

13.107.2 Constructor & Destructor Documentation

NonDIntegration ( ProblemDescDB & problem_db, Model & model ) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes
has been called and probDescDB can be queried for settings from the method specification. It is not currently
used, as there are not yet separate nond_quadrate/nond_sparse_grid method specifications.

References Dakota::abort_handler(), NonD::initialize_final_statistics(), NonD::initialize_random_variable_correlations(),
NonD::initialize_random_variable_transformation(), NonD::initialize_random_variable_types(), Analyzer::numDiscrete-IntVars,
Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, and NonD::verify_correlation_support().

NonDIntegration ( unsigned short method_name, Model & model ) [protected]

alternate constructor for instantiations "on the fly"

This alternate constructor is used for on-the-fly generation and evaluation of numerical integration points.
NonDIntegration ( unsigned short method_name, Model & model, const RealVector & dim_pref ) [protected]

alternate constructor for instantiations "on the fly"
    This alternate constructor is used for on-the-fly generation and evaluation of numerical integration points.

13.107.3 Member Function Documentation

void dimension_preference_to_anisotropic_order ( unsigned short scalar_order_spec, const RealVector & dim_pref_spec, size_t num_v, UShortArray & aniso_order ) [static]

convert scalar_order_spec and vector dim_pref_spec to vector aniso_order
    Converts a scalar order specification and a vector anisotropic dimension preference into an anisotropic order
    vector. It is used for initialization and does not enforce a reference lower bound (see also NonDQuadrature-::update_anisotropic_order()).
    Referenced by NonDPolynomialChaos::increment_specification_sequence(), NonDQuadrature::initialize_dimension_quadrature_order(), NonDPolynomialChaos::NonDPolynomialChaos(), and NonDPolynomialChaos::resize().

void anisotropic_order_to_dimension_preference ( const UShortArray & aniso_order, unsigned short & scalar_order, RealVector & dim_pref ) [static]

convert vector aniso_order to scalar_order and vector dim_pref
    Converts a vector anisotropic order into a scalar order and vector anisotropic dimension preference.
    Referenced by NonDPolynomialChaos::NonDPolynomialChaos().

void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
    Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
    Reimplemented from Iterator.
    References NonDIntegration::check_variables(), Analyzer::evaluate_parameter_sets(), Analyzer::get_parameter_sets(), Iterator::iteratedModel, NonD::natafTransform, and NonDIntegration::numIntegrations.

void check_variables ( const std::vector< Pecos::RandomVariable > & x_ran_vars ) [protected]

verify self-consistency of variables data
    Virtual function called from probDescDB-based constructors and from NonDIntegration::core_run()
    References Dakota::abort_handler(), NonD::numContAleatUncVars, NonD::numContDesVars, NonD::num-ContEpistUncVars, NonD::numContIntervalVars, Analyzer::numContinuousVars, and NonD::numContStateVars.
    Referenced by NonDIntegration::core_run(), NonDCubature::NonDCubature(), NonDQuadrature::NonDQuadrature(),
    and NonDSparseGrid::NonDSparseGrid().
    The documentation for this class was generated from the following files:
        • NonDIntegration.hpp
        • NonDIntegration.cpp

13.108 NonDInterval Class Reference

Base class for interval-based methods within DAKOTA/UQ.
    Inheritance diagram for NonDInterval:
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Public Member Functions

- **NonDInterval** (ProblemDescDB &problem_db, Model &model)
  *constructor*
- ~**NonDInterval** ()
  *destructor*
- void **print_results** (std::ostream &s)
  *print the cumulative distribution functions for belief and plausibility*
- bool **resize** ()
  *reinitializes iterator based on new variable size*

Protected Member Functions

- void **initialize_final_statistics** ()
  *initialize finalStatistics for belief/plausibility results sets*
- void **compute_evidence_statistics** ()
  *method for computing belief and plausibility values for response levels or vice-versa*
- void **calculate_cells_and_bpas** ()
  *computes the interval combinations (cells) and their bpas replaces CBPIIC_F77 from wrapper calculate_basic_prob_intervals()*
- void **calculate_cbf_cpf** (bool complementary=true)
  *function to compute (complementary) distribution functions on belief and plausibility replaces CCBFPF_F77 from wrapper calculate_cum_belief_plaus()*

Protected Attributes

- bool **singleIntervalFlag**
  *flag for SingleInterval derived class*
- RealVectorArray **ccBelFn**
  *Storage array to hold CCBF values.*
- RealVectorArray **ccPlausFn**
  *Storage array to hold CCPF values.*
- RealVectorArray **ccBelVal**
  *Storage array to hold CCB response values.*
- RealVectorArray **ccPlausVal**
  *Storage array to hold CCP response values.*
RealVectorArray cellContLowerBounds
  Storage array to hold cell lower bounds for continuous variables.

RealVectorArray cellContUpperBounds
  Storage array to hold cell upper bounds for continuous variables.

IntVectorArray cellIntRangeLowerBounds
  Storage array to hold cell lower bounds for discrete int range variables.

IntVectorArray cellIntRangeUpperBounds
  Storage array to hold cell upper bounds for discrete int range variables.

IntVectorArray cellIntSetBounds
  Storage array to hold cell values for discrete integer set variables.

IntVectorArray cellRealSetBounds
  Storage array to hold cell value for discrete real set variables.

RealVectorArray cellFnLowerBounds
  Storage array to hold cell min.

RealVectorArray cellFnUpperBounds
  Storage array to hold cell max.

RealVector cellBPA
  Storage array to hold cell bpa.

size_t respFnCntr
  response function counter

size_t cellCntr
  cell counter

size_t numCells
  total number of interval combinations

Additional Inherited Members

13.108.1 Detailed Description

Base class for interval-based methods within DAKOTA/UQ.

The NonDInterval class implements the propagation of epistemic uncertainty using either pure interval prop-
agation or Dempster-Shafer theory of evidence. In the latter approach, one assigns a set of basic probability
assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated,
along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response
surface is constructed which is sampled extensively to find the minimum and maximum within each input interval
cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to
calculate cumulative distribution functions for belief and plausibility.

The documentation for this class was generated from the following files:

- NonDInterval.hpp
- NonDInterval.cpp
13.109 NonDLHSEvidence Class Reference

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

Inheritance diagram for NonDLHSEvidence:

```
NonDLHSEvidence
  NonDLHSInterval
    NonDInterval
      NonD
        Analyzer
          Iterator
```

Public Member Functions

- NonDLHSEvidence (ProblemDescDB &problem_db, Model &model)
  
  constructor
- ~NonDLHSEvidence ()
  
  destructor
- void initialize ()
  
  perform any required initialization
- void post_process_samples ()
  
  post-process the output from executing lhsSampler

Additional Inherited Members

13.109.1 Detailed Description

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

The NonDEvidence class implements the propagation of epistemic uncertainty using Dempster-Shafer theory of evidence. In this approach, one assigns a set of basic probability assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated, along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response surface is constructed which is sampled extensively to find the minimum and maximum within each input interval cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to calculate cumulative distribution functions for belief and plausibility.

The documentation for this class was generated from the following files:

- NonDLHSEvidence.hpp
- NonDLHSEvidence.cpp
13.110 NonDLHSInterval Class Reference

Class for the LHS-based interval methods within DAKOTA/UQ.

Inheritance diagram for NonDLHSInterval:

```
NonDLHSInterval
   |       |
   v       v
NonDInterval
   |       |
   v       v
NonD
   |       |
   v       v
Analyzer
   |       |
   v       v
Iterator
```

Public Member Functions

- **NonDLHSInterval (ProblemDescDB &problem_db, Model &model)**
  
  *constructor*

- **~NonDLHSInterval ()**

  *destructor*

- **void derived_init_communicators (ParLevLIter pl_iter)**

  *derived class contributions to initializing the communicators associated with this Iterator instance*

- **void derived_set_communicators (ParLevLIter pl_iter)**

  *derived class contributions to setting the communicators associated with this Iterator instance*

- **void derived_free_communicators (ParLevLIter pl_iter)**

  *derived class contributions to freeing the communicators associated with this Iterator instance*

- **void core_run ()**

  *performs an epistemic uncertainty propagation using LHS samples*

Protected Member Functions

- **virtual void initialize ()**

  *perform any required initialization*

- **virtual void post_process_samples ()=0**

  *post-process the output from executing lhsSampler*
CHAPTER 13. CLASS DOCUMENTATION

Protected Attributes

- Iterator lhsSampler
  the LHS sampler instance
- const int seedSpec
  the user seed specification (default is 0)
- int numSamples
  the number of samples used
- String rngName
  name of the random number generator

Additional Inherited Members

13.110.1 Detailed Description

Class for the LHS-based interval methods within DAKOTA/UQ.
The NonDLHSInterval class implements the propagation of epistemic uncertainty using LHS-based methods.
The documentation for this class was generated from the following files:

- NonDLHSInterval.hpp
- NonDLHSInterval.cpp

13.111 NonDLHSSampling Class Reference

Performs LHS and Monte Carlo sampling for uncertainty quantification.
Inheritance diagram for NonDLHSSampling:

```
  Iterator
    Analyzer
      NonD
        NonDSampling
          NonDLHSSampling
```

Public Member Functions

- NonDLHSSampling (ProblemDescDB &problem_db, Model &model)
  standard constructor
- NonDLHSSampling (Model &model, unsigned short sample_type, int samples, int seed, const String &rng,
  bool vary_pattern=true, short sampling_vars_mode=ACTIVE)
  alternate constructor for sample generation and evaluation "on the fly"
• NonDLHSSampling (unsigned short sample_type, int samples, int seed, const String &rng, const RealVector &lower_bnds, const RealVector &upper_bnds)
  alternate constructor for uniform sample generation "on the fly"
• NonDLHSSampling (unsigned short sample_type, int samples, int seed, const String &rng, const RealVector &means, const RealVector &std_devs, const RealVector &lower_bnds, const RealVector &upper_bnds, RealSymMatrix &correl)
  alternate constructor for sample generation of correlated normals "on the fly"
• ~NonDLHSSampling ()
  destructor

Protected Member Functions
• void sampling_increment ()
  increment to next in sequence of refinement samples
• void pre_run ()
  generate LHS samples in non-VBD cases
• void core_run ()
  perform the evaluate parameter sets portion of run
• void post_run (std::ostream &s)
  generate statistics for LHS runs in non-VBD cases
• void post_input ()
  read tabular data for post-run mode
• void update_final_statistics ()
  update finalStatistics and (if MC sampling) finalStatErrors
• void compute_pca (std::ostream &s)
  compute a principal components analysis on the sample set
• void print_results (std::ostream &s)
  print the final statistics
• void d_optimal_parameter_set (int previous_samples, int new_samples, RealMatrix &full_samples)
  generate a d-optimal parameter set, leaving the first previous_samples columns intact and adding new_samples new columns following them
• void initial_increm_lhs_set (int new_samples, RealMatrix &full_samples, IntMatrix &full_ranks)
  Populate the first new_samples columns of allSamples with an LHS design and update the stored ranks.
• void increm_lhs_parameter_set (int previous_samples, int new_samples, RealMatrix &full_samples, IntMatrix &all_ranks)
  generate a new batch that is Latin w.r.t. the previous samples
• void store_ranks (const RealMatrix &sample_values, IntMatrix &sample_ranks)
  store the ranks of the last generated sample for continuous (based on sampleRanks) and calculate/store discrete ranks
• void store_ranks (IntMatrix &full_ranks)
  store the combined ranks from sampleRanks to leading submatrix local cached ranks matrix
• void combine_discrete_ranks (const RealMatrix &initial_values, const RealMatrix &increm_values)
  merge the discrete ranks into a submatrix of sampleRanks
Static Protected Member Functions

• static bool rank_sort (const int &x, const int &y)
  sort algorithm to compute ranks for rank correlations

Private Attributes

• size_t numResponseFunctions
  number of response functions; used to distinguish NonD from opt/NLS usage

• IntVector refineSamples
  list of refinement sample batch sizes

• bool dOptimal
  whether to generate d-optimal point sets

• size_t numCandidateDesigns
  number of candidate designs to generate for classical D-optimal designs

• Real oversampleRatio
  oversampling ratio for Leja D-optimal candidate set generation

• bool varBasedDecompFlag
  flags computation of variance-based decomposition indices

• bool pcaFlag
  flag to specify the calculation of principal components

• Real percentVarianceExplained
  Threshold to keep number of principal components that explain this much variance.

Static Private Attributes

• static RealArray rawData
  static data used by static rank_sort() fn

Additional Inherited Members

13.111.1 Detailed Description

Performs LHS and Monte Carlo sampling for uncertainty quantification.

The Latin Hypercube Sampling (LHS) package from Sandia Albuquerque’s Risk and Reliability organization provides comprehensive capabilities for Monte Carlo and Latin Hypercube sampling within a broad array of user-specified probabilistic parameter distributions. It enforces user-specified rank correlations through use of a mixing routine. The NonDLHSSampling class provides a C++ wrapper for the LHS library and is used for performing forward propagations of parameter uncertainties into response statistics.

Batch generation options, including D-Optimal and incremental LHS are provided.

The incremental LHS sampling capability allows one to supplement an initial sample of size n to size 2n while maintaining the correct stratification of the 2n samples and also maintaining the specified correlation structure. The incremental version of LHS will return a sample of size n, which when combined with the original sample of size n, allows one to double the size of the sample.
13.111 Constructor & Destructor Documentation

NonDLHSSampling (ProblemDescDB & problem_db, Model & model)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDLHSSampling::dOptimal, Model::num_primary_fns(), NonD::numBinomialVars, NonDLHSSampling::numCandidateDesigns, NonD::numDesignVars, NonD::numEpistemicUncVars, NonD::numGeometricVars, NonD::numHistogramPtIntVars, NonD::numHistogramPtRealVars, NonD::numHistogramPtStringVars, NonD::numHyperGeomVars, NonD::numNegBinomialVars, NonD::numPoissonVars, NonDLHSSampling::numResponseFunctions, NonD::numStateVars, Iterator::outputLevel, NonDLHSSampling::oversampleRatio, Model::primary_fn_type(), NonDLHSSampling::refineSamples, and NonDSampling::sampleType.

NonDLHSSampling (Model & model, unsigned short sample_type, int samples, int seed, const String & rng, bool vary_pattern = true, short sampling_vars_mode = ACTIVE)

alternate constructor for sample generation and evaluation "on the fly"

This alternate constructor is used for generation and evaluation of Model-based sample sets. A set_db_list_nodes has not been performed so required data must be passed through the constructor. It's purpose is to avoid the need for a separate LHS specification within methods that use LHS sampling.

NonDLHSSampling (unsigned short sample_type, int samples, int seed, const String & rng, const RealVector & lower_bnds, const RealVector & upper_bnds)

alternate constructor for uniform sample generation "on the fly"

This alternate constructor is used by ConcurrentStrategy for generation of uniform, uncorrelated sample sets. It is not a letter-envelope instantiation and a set_db_list_nodes has not been performed. It is called with all needed data passed through the constructor and is designed to allow more flexibility in variables set definition (i.e., relax connection to a variables specification and allow sampling over parameter sets such as multiobjective weights). In this case, a Model is not used and the object must only be used for sample generation (no evaluation).

References NonDSampling::get_parameter_sets().

NonDLHSSampling (unsigned short sample_type, int samples, int seed, const String & rng, const RealVector & means, const RealVector & std_devs, const RealVector & lower_bnds, const RealVector & upper_bnds, RealSymMatrix & correl)

alternate constructor for sample generation of correlated normals "on the fly"

This alternate constructor is used to generate correlated normal sample sets. It is not a letter-envelope instantiation and a set_db_list_nodes has not been performed. It is called with all needed data passed through the constructor. In this case, a Model is not used and the object must only be used for sample generation (no evaluation).

References NonDSampling::get_parameter_sets().

13.111.3 Member Function Documentation

void core_run() [protected], [virtual]

perform the evaluate parameter sets portion of run

Loop over the set of samples and compute responses. Compute statistics on the set of responses if statsFlag is set.
CHAPTER 13. CLASS DOCUMENTATION

Reimplemented from Iterator.
References NonDSampling::allDataFlag, Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, NonDLHSSampling::numResponseFunctions, and NonDSampling::statsFlag.

void d_optimal_parameter_set ( int previous_samples, int new_samples, RealMatrix & full_samples )
[protected]

generate a d-optimal parameter set, leaving the first previous_samples columns intact and adding new_samples new columns following them.

For now, when this function is called, numSamples is the number of new samples to generate.
References Model::aleatory_distribution_parameters(), Dakota::det_AtransA(), NonDSampling::get_parameter_sets(), Iterator::iteratedModel, NonDSampling::mode_counts(), NonD::natafTransform, NonDLHSSampling::numCandidateDesigns, Iterator::outputLevel, NonDLHSSampling::oversampleRatio, and NonDSampling::transform_samples().

Referenced by NonDLHSSampling::pre_run().
The documentation for this class was generated from the following files:

- NonDLHSSampling.hpp
- NonDLHSSampling.cpp

13.112 NonDLHSSingleInterval Class Reference

Class for pure interval propagation using LHS.

Inheritance diagram for NonDLHSSingleInterval:

```
   +-----------------+     +-----------------+
   | Iterator        |     | NonD             |
   +-----------------+     +-----------------+
         |                    +-----------------+  
         | Analyzer           |    | NonDInterval     |
   +-----------------+     +-----------------+  
         |                    +-----------------+  
         | NonDLHSSampling    |    | NonDLHSSingleInterval |
   +-----------------+                    +-----------------+
```

Public Member Functions

- **NonDLHSSingleInterval** (ProblemDescDB &problem_db, Model &model)
  *constructor*

- **~NonDLHSSingleInterval** ()
  *destructor*
13.113. **Nondlocalevidence Class Reference**

**Protected Member Functions**

- void initialize ()
  
  perform any required initialization
- void post_process_samples ()
  
  post-process the output from executing lhsSampler

**Private Attributes**

- size_t statCntr
  
  counter for finalStatistics

**Additional Inherited Members**

**Detailed Description**

Class for pure interval propagation using LHS.

The NonDSingleInterval class implements the propagation of epistemic uncertainty using ...

The documentation for this class was generated from the following files:

- NonDLHSSingleInterval.hpp
- NonDLHSSingleInterval.cpp

### 13.113 NonDLocalEvidence Class Reference

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

Inheritance diagram for NonDLocalEvidence:

```
    NonDLocalEvidence
     |                    |
     v                    v
  NonDLocalInterval      NonDInterval
     |                |                      |
     v                v                      v
  NonDLocalEvidence     NonDInterval     NonD
     |                      |                |
     v                      v              v
  Analyzer                NonD         NonDInterval
                                  |                |
                                  v              v
  Iterator
```

**Public Member Functions**

- **NonDLocalEvidence** (ProblemDescDB &problem_db, Model &model)
  
  constructor
- **~NonDLocalEvidence** ()
  
  destructor
Protected Member Functions

- void initialize ()
  perform any required initialization
- void set_cell_bounds ()
  set the optimization variable bounds for each cell
- void truncate_to_cell_bounds (RealVector &initial_pt)
  truncate initial_pt to respect current cell lower/upper bounds
- void post_process_cell_results (bool maximize)
  post-process a cell minimization/maximization result
- void post_process_response_fn_results ()
  post-process the interval computed for a response function
- void post_process_final_results ()
  perform final post-processing

Additional Inherited Members

13.113.1 Detailed Description

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

The NonDEvidence class implements the propagation of epistemic uncertainty using Dempster-Shafer theory of evidence. In this approach, one assigns a set of basic probability assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated, along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response surface is constructed which is sampled extensively to find the minimum and maximum within each input interval cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to calculate cumulative distribution functions for belief and plausibility.

The documentation for this class was generated from the following files:

- NonDLocalEvidence.hpp
- NonDLocalEvidence.cpp

13.114 NonDLocalInterval Class Reference

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDLocalInterval:
Public Member Functions

- **NonDLocalInterval (ProblemDescDB &problem_db, Model &model)**
  - constructor
- **~NonDLocalInterval ()**
  - destructor
- **void derived_init_communicators (ParLevLIter pl_iter)**
  - derived class contributions to initializing the communicators associated with this Iterator instance
- **void derived_set_communicators (ParLevLIter pl_iter)**
  - derived class contributions to setting the communicators associated with this Iterator instance
- **void derived_free_communicators (ParLevLIter pl_iter)**
  - derived class contributions to freeing the communicators associated with this Iterator instance
- **void core_run ()**
  - Performs a gradient-based optimization to determine interval bounds for an entire function or interval bounds on a particular statistical estimator.
- **unsigned short uses_method () const**
  - return name of active optimizer method
- **void method_recourse ()**
  - perform an MPP optimizer method switch due to a detected conflict

Protected Member Functions

- **virtual void initialize ()**
  - perform any required initialization
- **virtual void set_cell_bounds ()**
  - set the optimization variable bounds for each cell
- **virtual void truncate_to_cell_bounds (RealVector &initial_pt)**
  - truncate initial pt to respect current cell lower/upper bounds
- **virtual void post_process_cell_results (bool maximize)**
  - post-process a cell minimization/maximization result
virtual void post_process_response_fn_results ()
    post-process the interval computed for a response function
virtual void post_process_final_results ()
    perform final post-processing

Protected Attributes

- Iterator minMaxOptimizer
  local gradient-based optimizer
- Model minMaxModel
  recast model which extracts the active objective function

Static Private Member Functions

- static void extract_objective (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  static function used to extract the active objective function when optimizing for an interval lower or upper bound

Private Attributes

- bool npsolFlag
  flag representing the gradient-based optimization algorithm selection (NPSOL SQP or OPT++ NIP)

Static Private Attributes

- static NonDLocalInterval * nondLIInstance
  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

13.114.1 Detailed Description

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

The NonDLocalInterval class supports local gradient-based optimization approaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval analysis (e.g., intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels.

The documentation for this class was generated from the following files:

- NonDLocalInterval.hpp
- NonDLocalInterval.cpp
13.115 NonDLocalReliability Class Reference

Class for the reliability methods within DAKOTA/UQ.

Inheritance diagram for NonDLocalReliability:

```
NonDLocalReliability
    |________________________|
    |                           |
    |   NonDReliability         |
    |________________________|
    |                           |
    |   NonD                   |
    |________________________|
    |                           |
    |   Analyzer               |
    |________________________|
    |                           |
    |   Iterator               |
```

Public Member Functions

- **NonDLocalReliability (ProblemDescDB &problem_db, Model &model)**
  
  constructor

- **~NonDLocalReliability ()**
  
  destructor

- **void derived_init_communicators (ParLevLIter pl_iter)**
  
  derived class contributions to initializing the communicators associated with this Iterator instance

- **void derived_set_communicators (ParLevLIter pl_iter)**
  
  derived class contributions to setting the communicators associated with this Iterator instance

- **void derived_free_communicators (ParLevLIter pl_iter)**
  
  derived class contributions to freeing the communicators associated with this Iterator instance

- **void core_run ()**
  
  performs an uncertainty propagation using analytical reliability methods which solve constrained optimization problems to obtain approximations of the cumulative distribution function of response

- **void print_results (std::ostream &s)**
  
  print the approximate mean, standard deviation, and importance factors when using the mean value method or the CDF/CCDF information when using MPP-search-based reliability methods

- **unsigned short uses_method () const**
  
  return name of active MPP optimizer

- **void method_recourse ()**
  
  perform an MPP optimizer method switch due to a detected conflict

Private Member Functions

- **void initial_taylor_series ()**
  
  convenience function for performing the initial limit state Taylor-series approximation

- **void mean_value ()**
convenience function for encapsulating the simple Mean Value computation of approximate statistics and importance factors
• void mpp_search ()
  convenience function for encapsulating the reliability methods that employ a search for the most probable point
  (AMV, AMV+, FORM, SORM)
• void initialize_class_data ()
  convenience function for initializing class scope arrays
• void initialize_level_data ()
  convenience function for initializing/warm starting MPP search data for each response function prior to level 0
• void initialize_mpp_search_data ()
  convenience function for initializing/warm starting MPP search data for each z/p/beta level for each response function
• void mpp_search_data (const Variables &vars_star, const Response &resp_star)
  convenience function for updating MPP search data for each z/p/beta level for each response function
• void update_mpp_search_data ()
  convenience function for updating MPP search data for each z/p/beta level and final statistics following MPP convergence
• void update_limit_state_surrogate ()
  convenience function for passing the latest variables/response data to the data fit embedded within uSpaceModel
• void assign_mean_data ()
  update mostProbPointX/U, computedRespLevel, fnGradX/U, and fnHessX/U from ranVarMeansX/U, fnValsMeanX,
  fnGradsMeanX, and fnHessiansMeanX
• void dg_ds_eval (const RealVector &x_vars, const RealVector &fn_grad_x, RealVector &final_stat_grad)
  convenience function for evaluating dg/ds
• Real dp2_dbeta_factor (Real beta, bool cdf_flag)
  compute factor for derivative of second-order probability with respect to reliability index (from differentiating BR-
  EITUNG or HOHENRACK expressions)
• Real signed_norm (const RealVector &mpp_u, const RealVector &fn_grad_u, bool cdf_flag)
  convert norm of mpp_u (u-space solution) to a signed reliability index
• Real signed_norm (Real norm_mpp_u)
  convert norm of u-space vector to a signed reliability index
• Real signed_norm (Real norm_mpp_u, const RealVector &mpp_u, const RealVector &fn_grad_u, bool cdf_flag)
  shared helper function
• Real probability (Real beta)
  Convert reliability to probability using a first-order integration.
• Real probability (bool cdf_flag, const RealVector &mpp_u, const RealVector &fn_grad_u, const RealSym-
  Matrix &fn_hess_u)
  Convert computed reliability to probability using either a first-order or second-order integration.
• Real probability (Real beta, bool cdf_flag, const RealVector &mpp_u, const RealVector &fn_grad_u, const
  RealSymMatrix &fn_hess_u)
  Convert provided reliability to probability using either a first-order or second-order integration.
13.115. NONLOCALRELIABILITY CLASS REFERENCE

• Real reliability (Real \( p \))
  
  Convert probability to reliability using the inverse of a first-order integration.

• Real reliability (Real \( p \), bool cdf_flag, const RealVector &mpp_u, const RealVector &fn_grad_u, const RealSymMatrix &fn_hess_u)
  
  Convert probability to reliability using the inverse of a first-order or second-order integration.

• bool reliability_residual (const Real &p, const Real &beta, const RealVector &kappa, Real &res)
  
  Compute the residual for inversion of second-order probability corrections using Newton's method (called by reliability(p)).

• Real reliability residual_derivative (const Real &p, const Real &beta, const RealVector &kappa)
  
  Compute the residual derivative for inversion of second-order probability corrections using Newton's method (called by reliability(p)).

• void principal_curvatures (const RealVector &mpp_u, const RealVector &fn_grad_u, const RealSymMatrix &fn_hess_u, RealVector &kappa_u)
  
  Compute the \( \kappa_u \) vector of principal curvatures from \( \nabla^2 \).

• void scale_curvature (Real beta, bool cdf_flag, const RealVector &kappa, RealVector &scaled_kappa)
  
  Scale copy of principal curvatures by -1 if needed; else take a view

**Static Private Member Functions**

• static void RIA_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  
  Static function used as the objective function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of \( \| u \|^2 \).

• static void RIA_constraint_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  
  Static function used as the constraint function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the constraint of \( G(u) = \text{response level} \).

• static void PMA_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  
  Static function used as the objective function in the Performance Measure Approach (PMA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of \( G(u) \).

• static void PMA_constraint_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  
  Static function used as the constraint function in the first-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of \( \| u \|^2 = (\beta - \beta) \).

• static void PMA2_constraint_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)
  
  Static function used as the constraint function in the second-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of \( \beta = \beta - \beta \).

• static void PMA2_set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)
  
  Static function used to augment the sub-model ASV requests for second-order PMA
Private Attributes

- **Real computedRespLevel**
  - output response level calculated
- **Real computedRelLevel**
  - output reliability level calculated for RIA and 1st-order PMA
- **Real computedGenRelLevel**
  - output generalized reliability level calculated for 2nd-order PMA
- **RealVector fnGradX**
  - actual x-space gradient for current function from most recent response evaluation
- **RealVector fnGradU**
  - u-space gradient for current function updated from fnGradX and Jacobian dx/du
- **RealSymMatrix fnHessX**
  - actual x-space Hessian for current function from most recent response evaluation
- **RealSymMatrix fnHessU**
  - u-space Hessian for current function updated from fnHessX and Jacobian dx/du
- **RealVector kappaU**
  - principal curvatures derived from eigenvalues of orthonormal transformation of fnHessU
- **RealVector fnValsMeanX**
  - response function values evaluated at mean x
- **RealMatrix fnGradsMeanX**
  - response function gradients evaluated at mean x
- **RealSymMatrixArray fnHessiansMeanX**
  - response function Hessians evaluated at mean x
- **RealVector ranVarMeansX**
  - vector of means for all uncertain random variables in x-space
- **RealVector ranVarStdDevsX**
  - vector of std deviations for all uncertain random variables in x-space
- **RealVector ranVarMeansU**
  - vector of means for all uncertain random variables in u-space
- **bool initialPtUserSpec**
  - flag indicating user specification of (any portion of) initialPtU
- **RealVector initialPtUSpec**
  - user specification or default initial guess for local optimization
- **RealVector initialPtU**
  - current starting point for MPP searches in u-space
- **RealVector mostProbPointX**
  - location of MPP in x-space
- **RealVector mostProbPointU**
  - location of MPP in u-space
- **RealVectorArray prevMPPULev0**
  - array of converged MPP’s in u-space for level 0. Used for warm-starting initialPtU within RBDO.
- **RealMatrix prevFnGradDLev0**
matrix of limit state sensitivities w.r.t. inactive/design variables for level 0. Used for warm-starting initialPtU within RBDO.

- RealMatrix prevFnGradULev0

matrix of limit state sensitivities w.r.t. active/uncertain variables for level 0. Used for warm-starting initialPtU within RBDO.

- RealVector prevICVars

previous design vector. Used for warm-starting initialPtU within RBDO.

- ShortArray prevCumASVLev0

accumulation (using \(\|\cdot\|=\)) of all previous design ASV's from requested finalStatistics. Used to detect availability of prevFnGradDLev0 data for warm-starting initialPtU within RBDO.

- bool npsolFlag

flag representing the optimization MPP search algorithm selection (NPSOL SQP or OPT++ NIP)

- bool warmStartFlag

flag indicating the use of warm starts

- bool nipModeOverrideFlag

flag indicating the use of move overrides within OPT++ NIP

- bool curvatureDataAvailable

flag indicating that sufficient data (i.e., fnGradU, fnHessU, mostProbPointU) is available for computing principal curvatures

- bool kappaUpdated

track when kappaU requires updating via principal_curvatures()

- short integrationOrder

integration order (1 or 2) provided by integration specification

- short secondOrderIntType

type of second-order integration: Breitung, Hohenbichler-Rackwitz, or Hong

- Real curvatureThresh

cut-off value for \(1/\sqrt{\cdot}\) term in second-order probability corrections.

- short taylorOrder

order of Taylor series approximations (1 or 2) in MV/AMV/AMV+ derived from hessian type

- RealMatrix impFactor

importance factors predicted by MV

- int npsolDerivLevel

derivative level for NPSOL executions (1 = analytic grads of objective fn, 2 = analytic grads of constraints, 3 = analytic grads of both).

- unsigned short warningBits

set of warnings accumulated during execution

Static Private Attributes

- static NonDLocalReliability * nondLocRelInstance

pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data
Additional Inherited Members

13.115.1 Detailed Description

Class for the reliability methods within DAKOTA/UQ.

The NonDLocalReliability class implements the following reliability methods through the support of different limit state approximation and integration options: mean value (MVFOsM/MVSoS), advanced mean value method (AMV, AMV^2) in x- or u-space, iterated advanced mean value method (AMV+, AMV^2+) in x- or u-space, two-point adaptive nonlinearity approximation (TANA) in x- or u-space, first order reliability method (FORM), and second order reliability method (SORM). All options except mean value employ an optimizer (currently NPSOL SQP or OPT++ NIP) to solve an equality-constrained optimization problem for the most probable point (MPP). The MPP search may be formulated as the reliability index approach (RIA) for mapping response levels to reliabilities/probabilities or as the performance measure approach (PMA) for performing the inverse mapping of reliability/probability levels to response levels.

13.115.2 Member Function Documentation

void RIA_objective_eval ( const Variables & sub_model_vars, const Variables & recast_vars, const Response & sub_model_response, Response & recast_response ) [static], [private]

static function used as the objective function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of (norm u)^2.

This function recasts a G(u) response set (already transformed and approximated in other recursions) into an RIA objective function.

References Response::active_set_request_vector(), Variables::continuous_variables(), Response::function_gradient_view(), Response::function_hessian_view(), and Response::function_value().

Referenced by NonDLocalReliability::mpp_search().

void RIA_constraint_eval ( const Variables & sub_model_vars, const Variables & recast_vars, const Response & sub_model_response, Response & recast_response ) [static], [private]

static function used as the constraint function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the constraint of G(u) = response level.

This function recasts a G(u) response set (already transformed and approximated in other recursions) into an RIA equality constraint.

References Response::active_set_request_vector(), Response::function_gradient(), Response::function_gradient_view(), Response::function_hessian(), Response::function_value(), NonDLocalReliability::nondLocRelInstance, NonDReliability::requestedTargetLevel, and NonDReliability::respFnCount.

Referenced by NonDLocalReliability::mpp_search().

void PMA_objective_eval ( const Variables & sub_model_vars, const Variables & recast_vars, const Response & sub_model_response, Response & recast_response ) [static], [private]

static function used as the objective function in the Performance Measure Approach (PMA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of G(u).

This function recasts a G(u) response set (already transformed and approximated in other recursions) into a PMA objective function.
References

Response::active_set_request_vector(), Variables::continuous_variables(), NonDLocalReliability::curvatureDataAvailable, Response::function_gradient(), Response::function_gradient_view(), Response::function_hessian(), Response::function_hessian_view(), Response::function_value(), NonDLocalReliability::integrationOrder, NonDLocalReliability::kappaUpdated, NonReliability::mppSearchType, NonDLocalReliability::nondLocRelInstance, NonDReliability::pmaMaximizeG, NonDReliability::respFnCount, and NonDLocalReliability::update_pma_maximize().

Referenced by NonDLocalReliability::mpp_search().

```cpp
void PMA_constraint_eval ( const Variables & sub_model_vars, const Variables & recast_vars, const Response & sub_model_response, Response & recast_response ) [static], [private]
```

static function used as the constraint function in the first-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of \((\text{norm } u)^2 = (\beta - \bar{\beta})^2\).

This function recasts a \(G(u)\) response set (already transformed and approximated in other recursions) into a first-order PMA equality constraint on reliability index \(\beta\).

References

Response::active_set_request_vector(), Variables::continuous_variables(), Response::function_gradient_view(), Response::function_hessian_view(), Response::function_value(), NonDLocalReliability::nondLocRelInstance, and NonDReliability::requestedTargetLevel.

Referenced by NonDLocalReliability::mpp_search().

```cpp
void PMA2_constraint_eval ( const Variables & sub_model_vars, const Variables & recast_vars, const Response & sub_model_response, Response & recast_response ) [static], [private]
```

static function used as the constraint function in the second-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of \(\beta^* = \beta^* - \bar{\beta}\).

This function recasts a \(G(u)\) response set (already transformed and approximated in other recursions) into a second-order PMA equality constraint on generalized reliability index \(\beta^*\).

References

Dakota::abort_handler(), Response::active_set_request_vector(), NonD::cdfFlag, NonDLocalReliability::computedGenRelLevel, NonDLocalReliability::computedRelLevel, Variables::continuous_variables(), NonDLocalReliability::dp2_dbeta_factor(), NonDLocalReliability::fnGradU, NonDLocalReliability::fnHessU, Response::function_gradient_view(), Response::function_hessian(), Response::function_value(), NonDLocalReliability::mostProbPointU, NonDReliability::mppSearchType, NonDLocalReliability::nondLocRelInstance, NonDLocalReliability::probability(), NonDLocalReliability::reliability(), NonDReliability::respFnCount, and NonDLocalReliability::signed_norm().

Referenced by NonDLocalReliability::mpp_search().

```cpp
void initial_taylor_series( ) [private]
```

convenience function for performing the initial limit state Taylor-series approximation

An initial first- or second-order Taylor-series approximation is required for MV/AMV/AMV+/TANA or for the case where finalMomentStats (from MV) are required within finalStatistics for subIterator usage of NonDLocalReliability.

References

Response::active_set_request_vector(), Iterator::activeSet, Model::component_parallel_mode(), Model::continuous_variables(), Model::current_response(), Model::evaluate(), NonD::finalMomentsType, NonD::finalStatistics, NonDLocalReliability::fnGradsMeanX, NonDLocalReliability::fnHessiansMeanX, NonDLocalReliability::fnValsMeanX, Response::function_gradients(), Response::function_hessians(), Response::function_values(), Model::hessian_type(), Iterator::iteratedModel, NonDReliability::mppSearchType, NonD::natafTransform, Analyzer::numFunctions, NonD::numUncertainVars, NonDLocalReliability::ranVarMeansX, NonD-
LocalReliability::ranVarStdDevsX, ActiveSet::request_vector(), NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, Iterator::subIteratorFlag, NonDLocalReliability::taylorOrder, and NonDReliability::uSpaceModel.

Referenced by NonDLocalReliability::mean_value(), and NonDLocalReliability::mpp_search().

void initialize_class_data ( ) [private]
convenience function for initializing class scope arrays

Initialize class-scope arrays and perform other start-up activities, such as evaluating median limit state responses.

References Response::active_set_derivative_vector(), NonD::finalStatistics, NonDReliability::mppModel, NonD::natafTransform, Analyzer::numFunctions, NonDReliability::numRelAnalyses, NonD::numUncertainVars, NonDLocalReliability::prevCumASVLev0, NonDLocalReliability::prevFnGradDLLev0, NonDLocalReliability::prevFnGradDULev0, NonDLocalReliability::prevMPPULev0, NonDLocalReliability::ranVarMeansX, Iterator::subIteratorFlag, Model::update_from_subordinate_model(), and NonDLocalReliability::warmStartFlag.

Referenced by NonDLocalReliability::mpp_search().

void initialize_level_data ( ) [private]
convenience function for initializing/warm starting MPP search data for each response function prior to level 0

For a particular response function prior to the first z/p/beta level, initialize/warm-start optimizer initial guess (initialPtU), expansion point (mostProbPointX/U), and associated response data (computedRespLevel, fnGradX/U, and fnHessX/U).

References Iterator::activeSet, NonDLocalReliability::assign_mean_data(), Model::component_parallel_mode(), NonDLocalReliability::computedRespLevel, Model::continuous_variable_ids(), Model::continuous_variables(), Dakota::copy_data(), Model::current_response(), NonDLocalReliability::curvatureDataAvailable, Model::evaluate(), NonDLocalReliability::fnGradU, NonDLocalReliability::fnGradX, NonDLocalReliability::fnHessU, NonDLocalReliability::fnHessX, Response::function_gradient_copy(), Response::function_hessian(), Response::function_value(), Model::inactive_continuous_variables(), NonDLocalReliability::initialPtU, NonDLocalReliability::initialPtUSpec, Iterator::iteratedModel, NonDLocalReliability::kappaUpdated, NonDLocalReliability::mostProbPointU, NonDLocalReliability::mostProbPointX, NonDReliability::mppSearchType, NonD::natafTransform, NonDReliability::numRelAnalyses, NonD::numUncertainVars, NonDLocalReliability::prevCumASVLev0, NonDLocalReliability::prevFndGradDLLev0, NonDLocalReliability::prevFndGradDULev0, NonDLocalReliability::prevICVars, NonDLocalReliability::prevMPPLev0, ActiveSet::request_value(), ActiveSet::request_values(), NonD::requestedRespLevels, NonDReliability::respFnCount, Iterator::subIteratorFlag, Model::surrogate_function_indices(), NonDLocalReliability::taylorOrder, NonDLocalReliability::update_limit_state_surrogate(), NonDReliability::uSpaceModel, and NonDLocalReliability::warmStartFlag.

Referenced by NonDLocalReliability::mpp_search().

void initialize_mpp_search_data ( ) [private]
convenience function for initializing/warm starting MPP search data for each z/p/beta level for each response function

For a particular response function at a particular z/p/beta level, warm-start or reset the optimizer initial guess (initialPtU), expansion point (mostProbPointX/U), and associated response data (computedRespLevel, fnGradX/U, and fnHessX/U).

References NonDLocalReliability::assign_mean_data(), NonD::computedGenRelLevels, NonD::computedRelLevels, NonDLocalReliability::fnGradU, Model::hessian_type(), NonDLocalReliability::initialPtU, NonDLocalReliability::initialPtUSpec, NonDLocalReliability::integrationOrder, Iterator::iteratedModel, NonDReliability::level-
Count, NonDLocalReliability::mostProbPointU, NonDReliability::mppSearchType, NonD::numUncertainVars,
NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonDReliability::requested-
TargetLevel, NonDReliability::respFnCount, NonDLocalReliability::taylorOrder, and NonDLocalReliability::warm-
StartFlag.

Referenced by NonDLocalReliability::mpp_search().

```cpp
void update_mpp_search_data ( const Variables & vars_star, const Response & resp_star ) [private]
```

convenience function for updating MPP search data for each z/p/beta level for each response function

Includes case-specific logic for updating MPP search data for the AMV/AMV+/TANA/NO_APPROX methods.

References Response::active_set(), Response::active_set_request_vector(), Iterator::activeSet, NonDReliability-
::approxConverged, NonDReliability::approxIters, Model::component_parallel_mode(), NonDLocalReliability::computed-
RelLevel, NonDLocalReliability::computedRespLevel, Model::continuous_variable_ids(), Variables::continuous-
_variables(), Model::continuous_variables(), Iterator::convergenceTol, Variables::copy(), Dakota::copy_data(), Model-
::current_response(), Model::current_variables(), NonDLocalReliability::curvatureDataAvailable, Dakota::data-pairs,
Model::evaluate(), NonD::finalStatistics, NonDLocalReliability::fnGradU, NonDLocalReliability::fnGrad-
X, NonDLocalReliability::fnHessU, NonDLocalReliability::fnHessX, Response::function_derivative(), Response-
::function_hessian(), Response::function_value(), Response::function_values(), NonDLocalReliability::initialPu,
NonDLocalReliability::integrationOrder, Model::interface_id(), Iterator::iteratedModel, NonDLocalReliability::kappa-
Updated, NonDReliability::levelCount, Dakota::lookup_by_val(), Iterator::maxIters, NonDLocalReliability-
::mostProbPointU, NonDLocalReliability::mostProbPointX, NonDReliability::mppSearchType, NonD::natafTransform,
Analyzer::numFunctions, NonD::numNormalVars, NonD::numUncertainVars, NonDReliability::pmaMaximizeG,
ActiveSet::request_values(), ActiveSet::request_values(), ActiveSet::request_vector(), NonD::requestedProbLevels,
NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::requestedTargetLevel, NonDReliability-
::respFnCount, NonDLocalReliability::signed_norm(), NonDReliability::statCount, NonDLocalReliability::taylor-
Order, NonDLocalReliability::update_limit_state_surrogate(), NonDLocalReliability::update_pma_maximize(), Non-
DReliability::uSpaceModel, NonDLocalReliability::warmStartFlag, and NonDLocalReliability::warningBits.

Referenced by NonDLocalReliability::mpp_search().

```cpp
void update_level_data ( ) [private]
```

convenience function for updating z/p/beta level data and final statistics following MPP convergence

Updates computedRespLevels/computedProbLevels/computedRelLevels, finalStatistics, warm start, and graphics
data.

References Response::active_set_derivative_vector(), Response::active_set_request_vector(), Graphics::add_datapoint(),
NonD::cdfFlag, NonDLocalReliability::computedGenRelLevel, NonD::computedGenRelLevels, NonD::computed-
ProbLevels, NonD::computedRelLevel, NonD::computedRelLevels, NonDLocalReliability::computed-
RespLevel, NonD::computedRespLevels, NonDLocalReliability::computed-RelLevel, NonD::computedRespLevels, NonDLocalReliability::computed-
RespLevel, NonD::computedRespLevels, NonDLocalReliability::computed suspended(), NonDLocalReliability::dg_ds_eval(), NonDLocalReliability::dp2_dbeta-
_factor(), NonD::finalStatistics, NonDLocalReliability::fnGradU, NonDLocalReliability::fnGradX, NonDLocal-
Reliability::fnHessU, Response::function_derivative(), OutputManager::graphics(), NonDLocalReliability::integration-
Order, NonDReliability::levelCount, NonDLocalReliability::mostProbPointU, NonDLocalReliability::mostProb-
PointX, Graphics::new_dataset(), Analyzer::numFunctions, NonD::numUncertainVars, ParallelLibrary::output-
_manager(), Iterator::parallelLib, NonDLocalReliability::prevCumASVLev0, NonDLocalReliability::prevFnGrad-
DLev0, NonDLocalReliability::prevFnGradULev0, NonDLocalReliability::prevMPPULev0, NonDLocalReliability-
::probability(), NonDLocalReliability::reliability(), NonD::requestedGenRelLevels, NonD::requestedProbLevels,
NonD::requestedRelLevels, NonD::requestedRespLevels, NonDLocalReliability::respFnCount, NonD::respLevelTarget,
NonD::respLevelTargetReduce, NonDReliability::statCount, Iterator::subIteratorFlag, NonD::totalLevelRequests,
and NonDLocalReliability::warmStartFlag.

Referenced by NonDLocalReliability::mpp_search().
void dg_ds_eval ( const RealVector & x_vars, const RealVector & fn_grad_x, RealVector & final_stat_grad ) [private]

convenience function for evaluating dg/ds

Computes dg/ds where s = design variables. Supports potentially overlapping cases of design variable augmentation and insertion.

References Response::active_set_derivative_vector(), Iterator::activeSet, Model::all_continuous_variable_ids(), Model::component_parallel_mode(), Dakota::contains(), Model::continuous_variable_ids(), Model::continuous_variables(), Dakota::copy_data(), Model::current_response(), ActiveSet::derivative_vector(), Model::evaluate(), NonD::finalStatistics, Response::function_gradient_copy(), Response::function_gradients(), Model::inactive_continuous_variable_ids(), Iterator::iteratedModel, NonDReliability::mppSearchType, NonD::natafTransform, Iterator::primaryACVarMapIndices, ActiveSet::request_value(), ActiveSet::request_values(), NonDReliability::respFnCount, Iterator::secondaryACVarMapTargets, and NonDReliability::uSpaceModel.

Referenced by NonDLocalReliability::mean_value(), NonDLocalReliability::mpp_search(), and NonDLocalReliability::update_level_data().

Real dp2_dbeta_factor ( Real beta, bool cdf_flag ) [private]

compute factor for derivative of second-order probability with respect to reliability index (from differentiating BREITUNG or HOHENRACK expressions)

Compute sensitivity of second-order probability w.r.t. beta for use in derivatives of p^2 or beta* w.r.t. auxiliary parameters s (design, epistemic) or derivatives of beta* w.r.t. u in PMA2_constraint_eval().

References Dakota::abort_handler(), NonDLocalReliability::curvatureDataAvailable, NonDLocalReliability::curvatureThresh, NonDLocalReliability::kappaU, NonD::numUncertainVars, NonDLocalReliability::probability(), NonDLocalReliability::scale_curvature(), NonDLocalReliability::secondOrderIntType, and NonDLocalReliability::warningBits.

Referenced by NonDLocalReliability::PMA2_constraint_eval(), and NonDLocalReliability::update_level_data().

Real probability ( Real beta, bool cdf_flag, const RealVector & mpp_u, const RealVector & fn_grad_u, const RealSymMatrix & fn_hess_u ) [private]

Convert provided reliability to probability using either a first-order or second-order integration.

Converts beta into a probability using either first-order (FORM) or second-order (SORM) integration. The SORM calculation first calculates the principal curvatures at the MPP (using the approach in Ch. 8 of Haldar & Mahadevan), and then applies correction formulations from the literature (Breitung, Hohenbichler-Rackwitz, or Hong).

References NonDLocalReliability::curvatureDataAvailable, NonDLocalReliability::curvatureThresh, NonDAdaptImpSampling::final_probability(), NonDReliability::importanceSampler, NonDLocalReliability::integrationOrder, NonDReliability::integrationRefinement, Iterator::iterator_rep(), NonDLocalReliability::kappaU, NonDLocalReliability::kappaUpdated, NonDReliability::levelCount, Iterator::methodPCIter, NonD::miPLIndex, NonD::numUncertainVars, Iterator::outputLevel, NonDLocalReliability::principal_curvatures(), NonDLocalReliability::probability(), NonD::requestedRespLevels, NonDReliability::requestedTargetLevel, NonDReliability::respFnCount, Iterator::run(), NonDLocalReliability::scale_curvature(), NonDLocalReliability::secondOrderIntType, NonDLocalReliability::warningBits, and Dakota::write_precision.

The documentation for this class was generated from the following files:

- NonDLocalReliability.hpp
- NonDLocalReliability.cpp
13.116 NonDLocalSingleInterval Class Reference

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDLocalSingleInterval:

```
    NonDLocalSingleInterval
       |   
       v   
    NonDLocalInterval
       |   
       v   
    NonDInterval
       |   
       v   
    NonD
       |   
       v   
    Analyzer
       |   
       v   
    Iterator
```

Public Member Functions
- NonDLocalSingleInterval (ProblemDescDB &problem_db, Model &model) 
  constructor
- ~NonDLocalSingleInterval ()
  destructor

Protected Member Functions
- void initialize ()
  perform any required initialization
- void post_process_cell_results (bool maximize)
  post-process a cell minimization/maximization result

Private Attributes
- size_t statCntr
  counter for finalStatistics

Additional Inherited Members

13.116.1 Detailed Description

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

The NonDLocalSingleInterval class supports local gradient-based optimization approaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval
analysis (e.g. intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels.

The documentation for this class was generated from the following files:

- NonDLocalSingleInterval.hpp
- NonDLocalSingleInterval.cpp

13.117 NonDMultilevelSampling Class Reference

Performs Multilevel Monte Carlo sampling for uncertainty quantification.

Inheritance diagram for NonDMultilevelSampling:

```
   Iterator
    |
  Analyzer
    |
   NonD
    |
NonDSampling
    |
NonDMultilevelSampling
```

Public Member Functions

- **NonDMultilevelSampling (ProblemDescDB &problem_db, Model &model)**
  
  *standard constructor*

- **~NonDMultilevelSampling ()**
  
  *destructor*

- **bool resize ()**
  
  *reinitializes iterator based on new variable size*

Protected Member Functions

- **void pre_run ()**
  
  *pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori*

- **void core_run ()**

- **void post_run (std::ostream &s)**
  
  *post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way*

- **void print_results (std::ostream &s)**
  
  *print the final iterator results*
Private Member Functions

- void multilevel_mc_Ysum (size_t model_form)
  Perform multilevel Monte Carlo across the discretization levels for a particular model form using discrepancy accumulators (sum_Y)

- void multilevel_mc_Qsum (size_t model_form)
  Perform multilevel Monte Carlo across the discretization levels for a particular model form using QoI accumulators (sum_Q)

- void control_variate_mc (const SizetSizetPair &lf_form_level, const SizetSizetPair &hf_form_level)
  Perform control variate Monte Carlo across two model forms.

- void multilevel_control_variate_mc_Ycorr (size_t lf_model_form, size_t hf_model_form)
  Perform multilevel Monte Carlo across levels in combination with control variate Monte Carlo across model forms at each level; CV computes correlations for Y (LH correlations for level discrepancies)

- void multilevel_control_variate_mc_Qcorr (size_t lf_model_form, size_t hf_model_form)
  Perform multilevel Monte Carlo across levels in combination with control variate Monte Carlo across model forms at each level; CV computes correlations for Q (LH correlations for QoI)

- void shared_increment (size_t iter, size_t lev)
  perform a shared increment of LF and HF samples for purposes of computing/updating the evaluation ratio and the MSE ratio

- bool lf_increment (Real avg_eval_ratio, const SizetArray &N_lf, const SizetArray &N_hf, size_t iter, size_t lev)
  perform final LF sample increment as indicated by the evaluation ratio

- void load_pilot_sample (SizetArray &delta_N_l)
  distribute pilotSamples input across model forms or levels

- void load_pilot_sample (Sizet2DArray &delta_N_l)
  distribute pilotSamples input across model forms and levels

- void initialize_ml_Ysums (IntRealMatrixMap &sum_Y, size_t num_lev)
  initialize the ML accumulators for computing means, variances, and covariances across fidelity levels

- void initialize_ml_Qsums (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, IntIntPairRealMatrixMap &sum_QlQlm1, size_t num_lev)
  initialize the ML accumulators for computing means, variances, and covariances across fidelity levels

  initialize the CV accumulators for computing means, variances, and covariances across fidelity levels

  initialize the MLCV accumulators for computing means, variances, and covariances across fidelity levels

- void initialize_mlcv_sum (IntRealMatrixMap &sum_L1, IntRealMatrixMap &sum_L1m1, IntRealMatrixMap &sum_L1refined, IntRealMatrixMap &sum_L1m1refined, IntRealMatrixMap &sum_H1, IntRealMatrixMap &sum_H1m1, IntRealMatrixMap &sum_L1m1L1_L1m1, IntRealMatrixMap &sum_H1L1_L1m1, IntRealMatrixMap &sum_H1L1m1_L1m1, IntRealMatrixMap &sum_H1L1m1_L1m1, IntRealMatrixMap &sum_H1L1m1_L1m1, IntRealMatrixMap &sum_H1L1m1_L1m1, IntRealMatrixMap &sum_H1L1m1_L1m1, IntRealMatrixMap &sum_H1L1m1_L1m1, size_t num_ml_lev, size_t num_cv_lev)
  initialize the MLCV accumulators for computing means, variances, and covariances across fidelity levels

- void accumulate_ml_Qsums (IntRealMatrixMap &sum_Q, size_t levl, SizetArray &num_Q)
update running QoI sums for one model (sum_Q) using set of model evaluations within allResponses; used for level 0 from other accumulators

- void accumulate_ml_Ysums (IntRealMatrixMap &sum_Y, RealMatrix &sum_YY, size_t lev, SizetArray &num_Y)

  update accumulators for multilevel telescoping running sums using set of model evaluations within allResponses

- void accumulate_ml_Qsums (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, IntIntPairRealMatrixMap &sum_QlQlm1, size_t lev, SizetArray &num_Q)

  update running QoI sums for two models (sum_Ql, sum_Qlm1) using set of model evaluations within allResponses

- void accumulate_cv_Ysums (IntRealVectorMap &sum_L, SizetArray &num_L)

  update running sums for one model (sum_L) using set of model evaluations within allResponses


  update running sums for two models (sum_L, sum_H, and sum_LH) from set of low/high fidelity model evaluations within allResponses

- void accumulate_mlcv_Qsums (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, size_t lev, SizetArray &num_Q)

  update running QoI sums for one model at two levels (sum_Ql, sum_Qlm1) using set of model evaluations within allResponses

- void accumulate_mlcv_Ysums (IntRealMatrixMap &sum_Y, size_t lev, SizetArray &num_Y)

  update running discrepancy sums for one model (sum_Y) using set of model evaluations within allResponses


  update running QoI sums for two models (sum_L, sum_H, sum_LL, sum_LH, and sum_HH) from set of low/high fidelity model evaluations within allResponses


  update running two-level discrepancy sums for two models (sum_L, sum_H, sum_LL, sum_LH, and sum_HH) from set of low/high fidelity model evaluations within allResponses


  update running QoI sums for two models and two levels from set of low/high fidelity model evaluations within allResponses


  update running QoI sums for two models and two levels from set of low/high fidelity model evaluations within allResponses


  update running QoI sums for two models and two levels from set of low/high fidelity model evaluations within allResponses

- Real eval_ratio (const RealVector &sum_L_shared, const RealVector &sum_L, const RealVector &sum_H, const RealVector &sum_LL, const RealVector &sum_LH, Real cost_ratio, const SizetArray &N_shared, RealVector &var_H, RealVector &rhos_H)

  compute the LF/HF evaluation ratio, averaged over the QoI
• Real\ _eval\_ratio\ (RealMatrix &sum\_L\_shared, RealMatrix &sum\_H, RealMatrix &sum\_LL, RealMatrix &sum\_LH, RealMatrix &sum\_HH, Real cost\_ratio, size\_t lev, const SizetArray &N\_shared, RealMatrix &var\_H, RealMatrix &rho2\_LH)

  \textit{compute the LF/HF evaluation ratio, averaged over the QoI}

• Real\ _eval\_ratio\ (RealMatrix &sum\_L, RealMatrix &sum\_Ll, RealMatrix &sum\_Hl, RealMatrix &sum\_LLl, RealMatrix &sum\_LHl, RealMatrix &sum\_HHl, Real cost\_ratio, size\_t lev, const SizetArray &N\_shared, RealMatrix &var\_H, RealMatrix &rho2\_LH, RealMatrix &rho2\_LH)

  \textit{compute the LF/HF evaluation ratio, averaged over the QoI}

• Real\ _MSE\_ratio\ (Real avg\_eval\_ratio, const RealVector &var\_H, const RealVector &rho2\_LH, size\_t iter, const SizetArray &N\_hf)

  \textit{compute ratio of MC and CVMC mean squared errors, averaged over the QoI}


  \textit{compute control variate parameters for CVMC and estimate raw moments}


  \textit{apply control variate parameters for MLCVMC to estimate raw moment contributions}


  \textit{apply control variate parameters for MLCVMC to estimate raw moment contributions}

• void\ \texttt{compute\_control} (Real sum\_L, Real sum\_H, Real sum\_LL, Real sum\_LH, size\_t N\_shared, Real &beta)

  \textit{compute scalar control variate parameters}

• void\ \texttt{compute\_control} (Real sum\_L, Real sum\_H, Real sum\_LL, Real sum\_LH, Real \ sum\_HH, size\_t N\_shared, Real \ &var\_H, Real \ &rho2\_LH)

  \textit{compute scalar variance and correlation parameters for control variates}

• void\ \texttt{compute\_control} (Real sum\_L, Real sum\_Ll, Real sum\_Hl, Real sum\_ll, Real sum\_Ll\_Lm1, Real sum\_Ll\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Ll\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real sum\_Hl\_Lm1, Real \ &var\_YH, Real \ &rho2\_LH, Real \ &beta\_dot, Real \ &gamma)

  \textit{compute scalar control variate parameters}

• void\ \texttt{compute\_control} (const RealVector &sum\_L, const RealVector &sum\_H, const RealVector &sum\_LL, const RealVector &sum\_LH, const SizetArray &N\_shared, RealVector &beta)

  \textit{compute vector control variate parameters}

• void\ \texttt{compute\_control} (const RealVector &sum\_L, const RealVector &sum\_H, const RealVector &sum\_Ll, const RealVector &sum\_Lm1, const RealVector &sum\_Hl, const RealVector &sum\_LH, const RealVector &sum\_LHl, const RealVector &sum\_H, const RealVector \ &rho2\_LH)

  \textit{compute vector variance and correlation parameters for control variates}
void compute_control (const RealMatrix &sum_L, const RealMatrix &sum_H, const RealMatrix &sum_LL, const RealMatrix &sum_LH, const SizetArray &N_shared, size_t lev, RealVector &beta)

compute matrix control variate parameters

void compute_control (const RealMatrix &sum_Ll, const RealMatrix &sum_Llm1, const RealMatrix &sum_Hl, const RealMatrix &sum_Hlm1, const RealMatrix &sum_Ll_l, const RealMatrix &sum_Llm1_l, const RealMatrix &sum_Hl_l, const RealMatrix &sum_Hlm1_l, const RealMatrix &sum_Hl_Hl_m1, const RealMatrix &sum_Hl_Hlm1, const SizetArray &N_shared, size_t lev, RealVector &beta, RealVector &gamma)

compute matrix control variate parameters

void apply_control (Real sum_H, Real sum_L_shared, size_t N_shared, Real sum_L_refined, size_t N_refined, Real beta, Real &H_raw_mom)

apply scalar control variate parameter (beta) to approximate HF moment

void apply_control (Real sum_Hl, Real sum_Hlm1, Real sum_Ll, Real sum_Llm1, size_t N_shared, Real sum_Ll_refined, Real sum_Llm1_refined, size_t N_refined, Real beta_dot, Real gamma, Real &H_raw_mom)

apply scalar control variate parameter (beta) to approximate HF moment

void apply_control (const RealVector &sum_H, const RealVector &sum_L_shared, const SizetArray &N_shared, const RealVector &sum_L_refined, const SizetArray &N_refined, const RealVector &beta, RealVector &H_raw_mom)

apply vector control variate parameter (beta) to approximate HF moment

void apply_control (const RealMatrix &sum_H, const RealMatrix &sum_L_shared, const SizetArray &N_shared, const RealMatrix &sum_L_refined, const SizetArray &N_refined, size_t lev, const RealVector &beta, RealVector &H_raw_mom)

apply matrix control variate parameter (beta) to approximate HF moment

void apply_control (const RealMatrix &sum_H, const RealMatrix &sum_L_shared, const SizetArray &N_shared, const RealMatrix &sum_L_refined, const SizetArray &N_refined, size_t lev, const RealVector &beta, const RealVector &gamma, RealVector &H_raw_mom)

apply matrix control variate parameter (beta) to approximate HF moment

void export_all_samples (String root_prepend, const Model &model, size_t iter, size_t lev)

export allSamples to tagged tabular file

void convert_moments (const RealMatrix &raw_moments, RealMatrix &standard_moments)

convert uncentered raw moments (multilevel expectations) to standardized moments

void compute_error_estimates (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, IntIntPairRealMatrixMap &sum_QlQl, IntIntPairRealMatrixMap &sum_QlQlm1, Int2DArray &num_Q)

populate finalStatErrors for MLMC based on Q sums

Real aggregate_variance_Ysum (const Real *sum_Y, const Real *sum_YY, const SizetArray &N_l)

sum up variances across QoI (using sum_YY with means from sum_Y)

Real aggregate_variance_Qsum (const Real *sum_Ql, const Real *sum_Qlm1, const Real *sum_QlQl, const Real *sum_QlQlm1, const SizetArray &N_l, size_t lev)

sum up variances across QoI (using sum_YY with means from sum_Y)

Real aggregate_mse_Yvar (const Real *var_Y, const SizetArray &N_l)

sum up Monte Carlo estimates for mean squared error (MSE) across QoI using discrepancy variances

Real aggregate_mse_Ysum (const Real *sum_Y, const Real *sum_YY, const SizetArray &N_l)

sum up Monte Carlo estimates for mean squared error (MSE) across QoI using discrepancy sums
13.117. NONDMULTILEVELSAMPLING CLASS REFERENCE

- Real `aggregate_mse_Qsum` (const Real *sum_Ql, const Real *sum_QlQm1, const Real *sum_QlQl, const Real *sum_QlQlQm1, const Real &sum_QlQm1, const SizetArray &N_l, size_t lev)
  
  sum up Monte Carlo estimates for mean squared error (MSE) across QoI using discrepancy sums

- void `uncentered_to_centered` (Real rm1, Real rm2, Real rm3, Real rm4, Real &cm1, Real &cm2, Real &cm3, Real &cm4) const
  
  convert uncentered (raw) moments to centered moments

- void `centered_to_standard` (Real cm1, Real cm2, Real cm3, Real cm4, Real &sm1, Real &sm2, Real &sm3, Real &sm4) const
  
  convert centered moments to standardized moments

- Real `sum` (const Real *vec, size_t vec_len) const
  
  compute sum of a set of observations

- Real `average` (const Real *vec, size_t vec_len) const
  
  compute average of a set of observations

- Real `average` (const RealVector &vec) const
  
  compute average of a set of observations

- Real `average` (const SizetArray &sa) const
  
  compute average of a set of observations

- size_t `one_sided_delta` (Real current, Real target)
  
  compute a one-sided sample increment to move current sampling level to a new target

**Private Attributes**

- Sizet3DArray `NLev`
  
  total number of successful sample evaluations (excluding faults) for each model form, discretization level, and QoI

- SizetArray `pilotSamples`
  
  store the pilot samples input specification, prior to run-time invocation of `load_pilot_samples()`

- RealVector `mcMSEIter0`
  
  mean squared error of mean estimator from pilot sample MC on HF model

- Real `equivHFEvals`
  
  equivalent number of high fidelity evaluations accumulated using samples across multiple model forms and/or discretization levels

- bool `finalCVRefinement`
  
  if defined, complete the final CV refinement when terminating MLCV based on maxIterations (the total number of refinements beyond the pilot sample will be one more for CV than for ML). This approach is consistent with normal termination based on \|norm(delta_N_hf)\| = 0.

- bool `exportSampleSets`
  
  if defined, export each of the sample increments in ML, CV, MLCV using tagged tabular files

- unsigned short `exportSamplesFormat`
  
  format for exporting sample increments using tagged tabular files

**Additional Inherited Members**

13.117.1 Detailed Description

Performs Multilevel Monte Carlo sampling for uncertainty quantification.

Multilevel Monte Carlo (MLMC) is a variance-reduction technique that utilizes lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.
13.117.2 Constructor & Destructor Documentation

NonDMultilevelSampling ( ProblemDescDB & problem_db, Model & model )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, NonDMultilevelSampling::NLev, NonDMultilevelSampling::pilotSamples, NonDSampling::sampleType, Model::subordinate_models(), Model::surrogate_response_mode(), and Model::surrogate_type().

13.117.3 Member Function Documentation

void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s pre_run(), if implemented, typically before performing its own implementation steps.

Reimplemented from Analyzer.

References NonDMultilevelSampling::NLev, Analyzer::numFunctions, and Analyzer::pre_run().

void core_run ( ) [protected], [virtual]

The primary run function manages the general case: a hierarchy of model forms (from the ordered model fidelities within a HierarchSurrModel), each of which may contain multiple discretization levels.

Reimplemented from Iterator.

References NonDMultilevelSampling::control_variate_mc(), NonDMultilevelSampling::multilevel_control_variate_mc_Qcorr(), NonDMultilevelSampling::multilevel_control_variate_mc_Ycorr(), NonDMultilevelSampling::multilevel_mc_Qsum(), NonDMultilevelSampling::multilevel_mc_Ysum(), NonDMultilevelSampling::NLev, and Iterator::subIteratorFlag.

void post_run ( std::ostream & s ) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s post_run(), typically after performing its own implementation steps.

Reimplemented from Analyzer.

References Analyzer::post_run(), and NonDSampling::update_final_statistics().

void print_results ( std::ostream & s ) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References NonDMultilevelSampling::equivHFEvals, Iterator::iteratedModel, NonDMultilevelSampling::NLev, NonDSampling::print_moments(), NonD::print_multilevel_evaluation_summary(), Model::response_labels(), NonDSampling::statsFlag, and Model::truth_model().
void multilevel_mc_Ysum ( size_t model_form ) [private]
Perform multilevel Monte Carlo across the discretization levels for a particular model form using discrepancy accumulators (sum_Y).

This function performs "geometrical" MLMC on a single model form with multiple discretization levels.

References NonDMultilevelSampling::accumulate_ml_Ysums(), NonDMultilevelSampling::aggregate_mse_Ysum(), NonDMultilevelSampling::aggregate_variance_Ysum(), NonDMultilevelSampling::average(), Iterator::convergenceTol, NonDMultilevelSampling::convert_moments(), NonDMultilevelSampling::equivHFEvals, Analyzer::evaluate_parameter_sets(), NonDMultilevelSampling::export_all_samples(), NonDMultilevelSampling::exportSampleSets, NonD::finalMomentStats, NonDSampling::get_parameter_sets(), NonDMultilevelSampling::initialize_ml_Ysums(), Iterator::iteratedModel, NonDMultilevelSampling::load_pilot_sample(), Iterator::maxIterations, NonDMultilevelSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonDMultilevelSampling::one_sided_delta(), Iterator::outputLevel, Model::solution_level_cost(), Model::solution_levels(), Model::surrogate_model(), Model::surrogate_model_indices(), Model::truth_model(), and Model::truth_model_indices().

Referenced by NonDMultilevelSampling::core_run().

void multilevel_mc_Qsum ( size_t model_form ) [private]
Perform multilevel Monte Carlo across the discretization levels for a particular model form using QoI accumulators (sum_Q).

This function performs "geometrical" MLMC on a single model form with multiple discretization levels.

References NonDMultilevelSampling::accumulate_ml_Qsums(), NonDMultilevelSampling::aggregate_mse_Qsum(), NonDMultilevelSampling::aggregate_variance_Qsum(), NonDMultilevelSampling::average(), NonDMultilevelSampling::compute_error_estimates(), Iterator::convergenceTol, NonDMultilevelSampling::convert_moments(), NonDMultilevelSampling::equivHFEvals, Analyzer::evaluate_parameter_sets(), NonDMultilevelSampling::export_all_samples(), NonDMultilevelSampling::exportSampleSets, NonD::finalMomentStats, NonDSampling::get_parameter_sets(), NonDMultilevelSampling::initialize_ml_Qsums(), Iterator::iteratedModel, NonDMultilevelSampling::load_pilot_sample(), Iterator::maxIterations, NonDMultilevelSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonDMultilevelSampling::one_sided_delta(), Iterator::outputLevel, Model::solution_level_cost(), Model::solution_levels(), Model::surrogate_model(), Model::surrogate_model_indices(), Model::surrogate_response_mode(), and Model::truth_model().

Referenced by NonDMultilevelSampling::core_run().

void control_variate_mc ( const SizetSizetPair & lf_form_level, const SizetSizetPair & hf_form_level ) [private]
Perform control variate Monte Carlo across two model forms.

This function performs control variate MC across two combinations of model form and discretization level.

References NonDMultilevelSampling::accumulate_cv_sums(), Iterator::convergenceTol, NonDMultilevelSampling::convert_moments(), NonDMultilevelSampling::cv_raw_moments(), NonDMultilevelSampling::equivHFEvals, NonDMultilevelSampling::eval_ratio(), NonD::finalMomentStats, NonDMultilevelSampling::initialize_cv_sums(), Iterator::iteratedModel, NonDMultilevelSampling::lf_increment(), NonDMultilevelSampling::load_pilot_sample(), Iterator::maxIterations, NonDMultilevelSampling::MSE_ratio(), NonDMultilevelSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonDMultilevelSampling::shared_increment(), Model::solution_level_cost(), Model::surrogate_model(), Model::surrogate_model_indices(), Model::surrogate_response_mode(), Model::truth_model(), and Model::truth_model_indices().

Referenced by NonDMultilevelSampling::core_run().
void multilevel_control_variate_mc_Ycorr ( size_t lf_model_form, size_t hf_model_form ) [private]

Perform multilevel Monte Carlo across levels in combination with control variate Monte Carlo across model forms at each level; CV computes correlations for \( Y \) (LH correlations for level discrepancies)

This function performs "geometrical" MLMC across discretization levels for the high fidelity model form where CVMC si employed across two model forms to exploit correlation in the discrepancies at each level (\( Y_L \)).

References NonDMultilevelSampling::accumulate_ml_Ysums(), NonDMultilevelSampling::aggregate_mlcv_Ysums(), NonDMultilevelSampling::aggregate_mse_Ysum(), NonDMultilevelSampling::aggregate_mse_Yvar(), NonDMultilevelSampling::aggregate_variance_Ysum(), Analyzer::allResponses, NonDMultilevelSampling::average(), Iterator::convergenceTol, NonDMultilevelSampling::convert_moments(), NonDMultilevelSampling::cv_raw_moments(), NonDMultilevelSampling::eval_ratio(), Analyzer::evaluate_parameters_sets(), NonDMultilevelSampling::export_all_samples(), NonDMultilevelSampling::exportSampleSets, NonD::finalMomentsStats, NonDSampling::get_parameter_sets(), NonDMultilevelSampling::initialize_mlcv_sums(), Iterator::iteratedModel, NonDMultilevelSampling::lf_increment(), NonDMultilevelSampling::load_pilot_sample(), Iterator::maxIterations, NonDMultilevelSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonDMultilevelSampling::one_sided_delta(), Iterator::outputLevel, Model::solution_level_cost(), Model::solution_levels(), NonDMultilevelSampling::sum(), Model::surrogate_model(), Model::surrogate_model_indices(), Model::surrogate_response_mode(), Model::truth_model(), and Model::truth_model_indices().

Referenced by NonDMultilevelSampling::core_run().

void multilevel_control_variate_mc_Qcorr ( size_t lf_model_form, size_t hf_model_form ) [private]

Perform multilevel Monte Carlo across levels in combination with control variate Monte Carlo across model forms at each level; CV computes correlations for \( Q \) (LH correlations for QoI)

This function performs "geometrical" MLMC across discretization levels for the high fidelity model form where CVMC is employed across two model forms. It generalizes the \( Y_L \) correlation case to separately target correlations for each QoI level embedded within the level discrepancies.

References NonDMultilevelSampling::accumulate_ml_Ysums(), NonDMultilevelSampling::accumulate_mlcv_Qsums(), NonDMultilevelSampling::aggregate_mse_Ysum(), NonDMultilevelSampling::aggregate_mse_Yvar(), NonDMultilevelSampling::aggregate_variance_Ysum(), Analyzer::allResponses, NonDMultilevelSampling::average(), Iterator::convergenceTol, NonDMultilevelSampling::convert_moments(), NonDMultilevelSampling::cv_raw_moments(), NonDMultilevelSampling::eval_ratio(), Analyzer::evaluate_parameters_sets(), NonDMultilevelSampling::export_all_samples(), NonDMultilevelSampling::exportSampleSets, NonD::finalMomentsStats, NonDSampling::get_parameter_sets(), NonDMultilevelSampling::initialize_mlcv_sums(), Iterator::iteratedModel, NonDMultilevelSampling::lf_increment(), NonDMultilevelSampling::load_pilot_sample(), Iterator::maxIterations, NonDMultilevelSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonDMultilevelSampling::one_sided_delta(), Iterator::outputLevel, Model::solution_level_cost(), Model::solution_levels(), NonDMultilevelSampling::sum(), Model::surrogate_model(), Model::surrogate_model_indices(), Model::surrogate_response_mode(), Model::truth_model(), and Model::truth_model_indices().

Referenced by NonDMultilevelSampling::core_run().

The documentation for this class was generated from the following files:

- NonDMultilevelSampling.hpp
- NonDMultilevelSampling.cpp

13.118 NonDPOFDarts Class Reference

Base class for POF Dart methods within DAKOTA/UQ.

Inheritance diagram for NonDPOFDarts:
Public Member Functions

- **NonDPOFDarts (ProblemDescDB &problem_db, Model &model)**  
  *constructor*
- **~NonDPOFDarts ()**  
  *destructor*
- **bool resize ()**  
  *reinitializes iterator based on new variable size*
- **void core_run ()**  
  *perform POFDart analysis and return probability of failure*

Protected Member Functions

- **void initiate_random_number_generator (unsigned long x)**  
  *POF Darts Methods.*
- **double generate_a_random_number ()**
- **void init_pof_darts ()**
- **void exit_pof_darts ()**
- **void execute (size_t kd)**
- **void print_results (std::ostream &s)**  
  *print the final statistics*
- **void classical_dart_throwing_games (size_t game_index)**
- **void line_dart_throwing_games (size_t game_index)**
- **bool valid_dart (double *x)**
- **bool valid_line_flat (size_t flat_dim, double *flat_dart)**
- **void add_point (double *x)**
- **void compute_response (double *x)**
- **void verify_neighbor_consistency ()**
- **bool add_neighbor (size_t ipoint, size_t inneighbor)**
- **void retrieve_neighbors (size_t ipoint, bool update_point_neighbors)**
- **void sample_furthest_vertex (size_t ipoint, double *fv)**
- **void update_global_L ()**
- **void assign_sphere_radius_POF (size_t isample)**
- **void shrink_big_spheres ()**
- **double area_triangle (double x1, double y1, double x2, double y2, double x3, double y3)**
void initialize_surrogates()
void add_surrogate_data (const Variables &vars, const Response &resp)
void build_surrogate()
double eval_surrogate (size_t fn_index, double *vin)
void estimate_pof_surrogate()
bool trim_line_using_Hyperplane (size_t num_dim, double *st, double *end, double *qH, double *nH)
double f_true (double *x)
void plot_vertices_2d (bool plot_true_function, bool plot_surrogate)
void plot_neighbors ()

Protected Attributes

- int samples
- int seed
- int emulatorSamples
- String lipschitzType
- RealRealPairArray extremeValues
- double Q [1220]
- int index
- double cc
- double c
- double zc
- double zx
- double zy
- size_t qlen
- bool _eval_error
- size_t _test_function
- size_t _n_dim
- double * _xmin
- double * _xmax
- double _diag
- double _failure_threshold
- double _num_darts
- double _num_successive_misses_p
- double _num_successive_misses_m
- double _max_num_successive_misses
- double _accepted_void_ratio
- size_t _num_inserted_points
- size_t _total_budget
- double ** _sample_points
- size_t ** _sample_neighbors
- double * _sample_vsize
- double _max_vsize
- double * _dart
- size_t _flat_dim
- size_t * _line_flat
- size_t _num_flat_segments
13.119 NonDPolynomialChaos Class Reference

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

Inheritance diagram for NonDPolynomialChaos:

```
NonD PolynomialChaos
NonDExpansion
NonD
Analyzer
Iterator
```

Public Member Functions

- **NonDPolynomialChaos** (ProblemDescDB &problem_db, Model &model)
  
  *standard constructor*
• **NonDPolynomialChaos** (Model &model, short exp_coeffs_approach, const UShortArray &num_int_seq, const RealVector &dim_pref, short u_space_type, bool piecewise_basis, bool use_derivs)
  alternate constructor for numerical integration (tensor, sparse, cubature)

• **NonDPolynomialChaos** (Model &model, short exp_coeffs_approach, const UShortArray &exp_order_seq, const RealVector &dim_pref, const SizetArray &colloc_pts_seq, Real colloc_ratio, int seed, short u_space_type, bool piecewise_basis, bool use_derivs, bool cv_flag, const String &import_build_points_file, unsigned short import_build_format, bool import_build_active_only)
  alternate constructor for regression (least squares, CS, OLI)

• ~NonDPolynomialChaos ()
  destructor

• bool resize ()
  reinitializes iterator based on new variable size

### Protected Member Functions

• void derived_init_communicators (ParLevLIter pl_iter)
  derived class contributions to initializing the communicators associated with this Iterator instance

• void derived_set_communicators (ParLevLIter pl_iter)
  derived class contributions to setting the communicators associated with this Iterator instance

• void derived_free_communicators (ParLevLIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance

• void resolve_inputs (short &u_space_type, short &data_order)
  perform error checks and mode overrides

• void initialize_u_space_model ()
  initialize uSpaceModel polynomial approximations with PCE/SC data

• void increment_specification_sequence ()
  increment the input specification sequence (PCE only)

• void compute_expansion ()
  form or import an orthogonal polynomial expansion using PCE methods

• void multifidelity_expansion ()
  construct a multifidelity expansion, across model forms or discretization levels

• void select_refinement_points (const RealVectorArray &candidate_samples, unsigned short batch_size, RealMatrix &best_samples)
  evaluate allSamples for inclusion in the (PCE regression) approximation and retain the best set (well spaced) of size batch_size

• void select_refinement_points Deprecated (const RealVectorArray &candidate_samples, unsigned short batch_size, RealMatrix &best_samples)

• void append_expansion (const RealMatrix &samples, const IntResponseMap &resp_map)
  append new data to uSpaceModel and update expansion order (PCE only)

• void increment_order_and_grid ()

• void print_results (std::ostream &s)
  print the final coefficients and final statistics

• void print_coefficients (std::ostream &s)
  print the PCE coefficient array for the orthogonal basis

• void archive_coefficients ()
archive the PCE coefficient array for the orthogonal basis

- void multilevel_regression (size_t model_form)
  special case of multifidelity_expansion() for multilevel allocation of samples, mirroring NonDMultilevelSampling for least sq/compressed sensing

- void increment_sample_sequence (size_t new_samp, size_t total_samp)
  increment the sequence in numSamplesOnModel for multilevel_regression()

- void append_expansion ()
  generate new samples from numSamplesOnModel and update expansion

Private Member Functions

- void increment_grid_from_order ()
  define a grid increment that is consistent with an advancement in expansion order

- void increment_order_from_grid ()
  define an expansion order that is consistent with an advancement in structured/unstructured grid level/density

- int terms_ratio_to_samples (size_t num_exp_terms, Real colloc_ratio)
  convert number of expansion terms and collocation ratio to a number of collocation samples

- Real terms_samples_to_ratio (size_t num_exp_terms, int samples)
  convert number of expansion terms and number of collocation samples to a collocation ratio

- void ratio_samples_to_order (Real colloc_ratio, int num_samples, UShortArray &exp_order, bool less_than_or_equal)
  convert collocation ratio and number of samples to expansion order

- void order_to_dim_preference (const UShortArray &order, unsigned short &p, RealVector &dim_pref)
  convert an isotropic/anisotropic expansion_order vector into a scalar plus a dimension preference vector

Private Attributes

- String expansionExportFile
  filename for export of chaos coefficients

- String expansionImportFile
  filename for import of chaos coefficients

- Real collocRatio
  factor applied to terms^termsOrder in computing number of regression points, either user specified or inferred

- Real termsOrder
  exponent applied to number of expansion terms for computing number of regression points

- int randomSeed
  seed for random number generator used for regression with LHS and sub-sampled tensor grids

- bool tensorRegression
  option for regression PCE using a filtered set tensor-product points

- bool crossValidation
  flag for use of cross-validation for selection of parameter settings in regression approaches

- bool crossValidNoiseOnly
  flag to restrict cross-validation to only estimate the noise tolerance in order to manage computational cost

- RealVector noiseTols
• **Real** `l2Penalty`
  
  $L_2$ penalty for LASSO algorithm (elastic net variant)

• **unsigned short** `numAdvance`
  
  number of frontier expansions per iteration with the ADAPTED BASIS EXPANDING FRONT approach

• **USHortArray** `expOrderSeqSpec`
  
  user specification for expansion order (array for multifidelity)

• **RealVector** `dimPrefSpec`
  
  user specification for dimension preference

• **SizetArray** `collocPtsSeqSpec`
  
  user specification for collocation points (array for multifidelity)

• **SizetArray** `expSamplesSeqSpec`
  
  user specification for expansion samples (array for multifidelity)

• **size_t** `sequenceIndex`
  
  sequence index for `{expOrder,collocPts,expSamples}` SeqSpec

• **RealMatrix** `pceGradsMeanX`
  
  derivative of the PCE with respect to the x-space variables evaluated at the means (used as uncertainty importance metrics)

• **bool** `normalizedCoeffOutput`
  
  user request for use of normalization when outputting PCE coefficients

• **short** `uSpaceType`
  
  user requested expansion type

• **USHortArray** `quadOrderSeqSpec`
  
  user request of quadrature order

• **USHortArray** `ssgLevelSeqSpec`
  
  user request of sparse grid level

• **unsigned short** `cubIntSpec`
  
  cubature integrand

• **String** `importBuildPointsFile`
  
  user specified import build points file

• **unsigned short** `importBuildFormat`
  
  user specified import build file format

• **bool** `importBuildActiveOnly`
  
  user specified import build active only

• **String** `importApproxPointsFile`
  
  user specified import approx. points file

• **unsigned short** `importApproxFormat`
  
  user specified import approx. file format

• **bool** `importApproxActiveOnly`
  
  user specified import approx. active only

• **SizetArray** `NLev`
  
  number of samples allocated to each level of a discretization hierarchy within multilevel regression

• **Real** `equivHEvals`
  
  equivalent number of high fidelity evaluations accumulated using samples across multiple model forms and/or discretization levels
Additional Inherited Members

13.119.1 Detailed Description

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

The NonDPolynomialChaos class uses a polynomial chaos expansion (PCE) approach to approximate the
effect of parameter uncertainties on response functions of interest. It utilizes the OrthogPolyApproximation class
to manage multiple types of orthogonal polynomials within a Wiener-Askey scheme to PCE. It supports PCE
coefficient estimation via sampling, quadrature, point-collocation, and file import.

13.119.2 Constructor & Destructor Documentation

NonDPolynomialChaos ( ProblemDescDB & problem_db, Model & model )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Dakota::abort_handler(), Response::active_set(), NonDIntegration::anisotropic_order_to_dimension-
_preference(), Model::assign_rep(), NonDExpansion::check_dimension_preference(), NonDPolynomialChaos::colloc-
PtsSeqSpec, NonDPolynomialChaos::collocRatio, ParallelLibrary::command_line_check(), NonDExpansion::construct-
cubature(), NonDExpansion::construct_expansion_sampler(), NonD::construct_lhs(), NonDExpansion::construct-
quadrature(), NonDPolynomialChaos::cubIntSpec, Model::current_response(), NonDIntegration::dimension_preference_to_anisotropic_order(), NonDPolynomialChaos::dimPrefSpec, NonDExpansion::expansionBasisType, NonDExpansion::expansionCoeffsApproach, NonDPolynomialChaos::expansionImportFile, NonDPolynomialChaos::expOrderSeqSpec, NonDPolynomialChaos::expSamplesSeqSpec, ProblemDescDB::get_real(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::get_usa(), ProblemDescDB::get_ushort(), NonDPolynomialChaos::importApproxActiveOnly, NonDPolynomialChaos::importApproxFormat, NonDPolynomialChaos::importApproxPointsFile, NonDPolynomialChaos::importBuildActiveOnly, NonDPolynomialChaos::importBuildFormat, NonDPolynomialChaos::importBuildPointsFile, NonDExpansion::initialize(), NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, Analyzer::numContinuousVars, NonDExpansion::numSamplesOnModel, Iterator::outputLevel, Iterator::parallelLib, Iterator::probDescDB, NonDPolynomialChaos::quadOrderSeqSpec, NonDPolynomialChaos::randomSeed, NonDExpansion::refineControl, NonDExpansion::refineType, ActiveSet::request_values(), NonDPolynomialChaos::resolve_inputs(), NonDPolynomialChaos::sequenceIndex, NonDPolynomialChaos::ssgLevelSeqSpec, NonDPolynomialChaos::tensor-Regression, NonDPolynomialChaos::terms_ratio_to_samples(), NonDPolynomialChaos::terms_samples_to_ratio(), NonDPolynomialChaos::termsOrder, NonD::transform_model(), NonDExpansion::uSpaceModel, NonDPolynomial-Chaos::uSpaceType, and Analyzer::vary_pattern().

NonDPolynomialChaos ( Model & model, short exp_coeffs_approach, const UShortArray & num_int_seq,
const RealVector & dim_pref, short u_space_type, bool piecewise_basis, bool use_derivs )

alternate constructor for numerical integration (tensor, sparse, cubature)

This constructor is used for helper iterator instantiation on the fly that employ numerical integration (quadra-
ture, sparse grid, cubature).

References Response::active_set(), Model::assign_rep(), NonDExpansion::check_dimension_preference(), NonDExpansion::construct_cubature(), NonDExpansion::construct_quadrature(), NonDExpansion::construct_sparse_grid(), Model::current_response(), NonDPolynomialChaos::dimPrefSpec, NonDExpansion::expansionCoeffsApproach, NonDExpansion::initialize(), NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, ActiveSet::request_values(), NonDPolynomialChaos::resolve_inputs(), NonD::transform_model(), NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.
alternate constructor for regression (least squares, CS, OLI)

This constructor is used for helper iterator instantiation on the fly that employ regression (least squares, CS, OLI).

References Response::active_set(), Model::assign_rep(), NonDExpansion::check_dimension_preference(), NonDPolynomialChaos::collocPtsSeqSpec, NonDPolynomialChaos::collocRatio, NonD::construct_lhs(), NonDExpansion::construct_quadrature(), Model::current_response(), NonDIntegration::dimension_preference_to_anisotropic_order(), NonDPolynomialChaos::dimPrefSpec, NonDExpansion::expansionBasisType, NonDPolynomialChaos::expOrder_SeqSpec, NonDExpansion::initialize(), NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, Analyzer::numContinuousVars, NonDExpansion::numSamplesOnModel, Iterator::outputLevel, NonDPolynomialChaos::randomSeed, ActiveSet::request_values(), NonDPolynomialChaos::resolve_inputs(), NonDPolynomialChaos::sequenceIndex, NonDPolynomialChaos::tensorRegression, NonDPolynomialChaos::terms_ratio_to_samples(), NonD::transform_model(), NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.

13.119.3 Member Function Documentation

void increment_specification_sequence ( ) [protected], [virtual]

increment the input specification sequence (PCE only)

default implementation is overridden by PCE

Reimplemented from NonDExpansion.

References NonDPolynomialChaos::collocPtsSeqSpec, NonDPolynomialChaos::collocRatio, SharedApproxData::data_rep(), NonDIntegration::dimension_preference_to_anisotropic_order(), NonDPolynomialChaos::dimPrefSpec, SharedPecosApproxData::expansion_order(), NonDExpansion::expansionBasisType, NonDExpansion::expansion_CoeffsApproach, NonDPolynomialChaos::expOrder_SeqSpec, NonDExpansion::expSamplesSeqSpec, NonDExpansion::increment_specification_sequence(), Iterator::iterator_rep(), NonDQuadrature::mode(), Model::model_rep(), Analyzer::numContinuousVars, NonDExpansion::numSamplesOnModel, NonDQuadrature::quadrature_order(), NonDQuadrature::samples(), Iterator::sampling_reference(), NonDPolynomialChaos::sequenceIndex, Model::shared_approximation(), Model::subordinate_iterator(), NonDPolynomialChaos::tensorRegression, NonDPolynomialChaos::terms_ratio_to_samples(), DataFitSurrModel::total_points(), NonDQuadrature::update(), and NonDExpansion::uSpaceModel.

void increment_order_and_grid ( ) [protected], [virtual]

Used for uniform refinement of regression-based PCE.

Reimplemented from NonDExpansion.

References SharedApproxData::data_rep(), NonDPolynomialChaos::increment_grid_from_order(), SharedPecosApproxData::increment_order(), Model::shared_approximation(), and NonDExpansion::uSpaceModel.

void increment_grid_from_order ( ) [private]

define a grid increment that is consistent with an advancement in expansion order

Used for uniform refinement of regression-based PCE.

References NonDPolynomialChaos::collocRatio, SharedApproxData::data_rep(), SharedPecosApproxData::expansion_order(), NonDExpansion::expansionBasisType, NonDQuadrature::increment_grid(), Iterator::iterator_rep(), NonDQuadrature::mode(), Model::model_rep(), NonDExpansion::numSamplesOnModel, NonDQuadrature::samples(), Iterator::sampling_reference(), Model::shared_approximation(), Model::subordinate_iterator(), Non-
DPolynomialChaos::tensorRegression, NonDPolynomialChaos::terms_ratio_to_samples(), DataFitSurrModel::total_points(), NonDQuadrature::update(), and NonDExpansion::uSpaceModel.

Referenced by NonDPolynomialChaos::increment_order_and_grid().

```cpp
void increment_order_from_grid() [private]
```

define an expansion order that is consistent with an advancement in structured/unstructured grid level/density

Used for uniform refinement of regression-based PCE.

References NonDPolynomialChaos::collocRatio, SharedApproxData::data_rep(), SharedPecosApproxData::expansion_order(), NonDExpansion::numSamplesOnModel, NonDPolynomialChaos::ratio_samples_to_order(), Model::shared_approximation(), and NonDExpansion::uSpaceModel.

Referenced by NonDPolynomialChaos::append_expansion().

The documentation for this class was generated from the following files:

- NonDPolynomialChaos.hpp
- NonDPolynomialChaos.cpp

### 13.120 NonDQuadrature Class Reference

Derived nondeterministic class that generates N-dimensional numerical quadrature points for evaluation of expectation integrals over uncorrelated standard normals/uniforms/exponentials/betas/gammas.

Inheritance diagram for NonDQuadrature:

```
     Iterator
      /     \
    /       \
  Analyzer     \
     |       \
    | NonD    \
  NonDIntegration
      |     \
      | NonDQuadrature
```

### Public Member Functions

- **NonDQuadrature (Model &model, const UShortArray &quad_order_seq, const RealVector &dim_pref, short driver_mode)**
  
  *alternate constructor for instantiations "on the fly" based on a quadrature order specification*

- **NonDQuadrature (Model &model, int num_filt_samples, const RealVector &dim_pref, short driver_mode)**

  *alternate constructor for instantiations "on the fly" that generate a filtered tensor product sample set*

- **NonDQuadrature (Model &model, int num_rand_samples, int seed, const UShortArray &quad_order_seq, const RealVector &dim_pref, short driver_mode)**

  *alternate constructor for instantiations "on the fly" that sample randomly from a tensor product multi-index*

- **void increment_grid()**
increment SSG level/TPQ order

- **void update ()**
  
  propagate any numSamples updates and/or grid updates/increments

- **const Pecos::UShortArray & quadrature_order () const**
  
  return Pecos::TensorProductDriver::quadOrder

- **void quadrature_order (const Pecos::UShortArray &dim_quad_order)**
  
  set dimQuadOrderRef and map to Pecos::TensorProductDriver::quadOrder

- **void samples (size_t samples)**
  
  set numSamples

- **short mode () const**
  
  return quadMode

**Protected Member Functions**

- **NonDQuadrature (ProblemDescDB &problem_db, Model &model)**
  
  constructor

- **~NonDQuadrature ()**
  
  destructor

- **void initialize_grid (const std::vector<Pecos::BasisPolynomial> &poly_basis)**
  
  Generate one block of numSamples samples (ndim * num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.

- **void reset ()**
  
  restore initial state for repeated sub-iterator executions

- **void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)**

- **void increment_grid_preference (const RealVector &dim_pref)**
  
  increment SSG level/TPQ order and update anisotropy

- **void increment_specification_sequence ()**
  
  increment sequenceIndex and update active orders/levels

- **int num_samples () const**

**Private Member Functions**

- **void increment_grid (UShortArray &dim_quad_order)**
  
  convenience function used to make increment_grid() more modular

- **void increment_grid_preference (const RealVector &dim_pref, UShortArray &dim_quad_order)**
  
  convenience function used to make increment_grid_preference() more modular

- **void compute_minimum_quadrature_order (size_t min_samples, const RealVector &dim_pref, UShortArray &dim_quad_order)**
  
  calculate smallest dim_quad_order with at least min_samples

- **void filter_parameter_sets ()**
  
  prune allSamples back to size numSamples, retaining points with highest product weight

- **void update_anisotropic_order (const RealVector &dim_pref, UShortArray &quad_order_ref)**
  
  update quad_order_ref based on an updated dimension preference, enforcing previous values as a lower bound
13.120. NONDQUADRATURE CLASS REFERENCE

- void `initialize_dimension_quadrature_order` (unsigned short `quad_order_spec`, const `RealVector &dim_pref_spec`, `UShortArray &dim_quad_order`)
  
  initialize `dim_quad_order` from `quad_order_spec` and `dim_pref_spec`

- void `increment_dimension_quadrature_order` (`UShortArray &dim_quad_order`)

  increment each `dim_quad_order` entry by 1

- void `increment_dimension_quadrature_order` (const `RealVector &dim_pref`, `UShortArray &dim_quad_order`)

  increment the `dim_quad_order` entry with maximum preference by 1 and then rebalance

**Private Attributes**

- `Pecos::TensorProductDriver * tpqDriver`

  convenience pointer to the numIntDriver representation

- bool `nestedRules`

  for studies involving refinement strategies, allow for use of nested quadrature rules such as Gauss-Patterson

- `UShortArray quadOrderSeqSpec`

  a sequence of scalar quadrature orders, one per refinement level

- `UShortArray dimQuadOrderRef`

  reference point for `Pecos::TensorProductDriver::quadOrder`: the original user specification for the number of Gauss points per dimension, plus any refinements posted by `increment_grid`

- short `quadMode`

  point generation mode: FULL_TENSOR, FILTERED_TENSOR, RANDOM_TENSOR

- `size_t numSamples`

  size of a subset of tensor quadrature points (filtered based on product weight or sampled uniformly from the tensor multi-index); used by the regression PCE approach known as "probabilistic collocation"

- int `randomSeed`

  seed for the random number generator used in sampling of the tensor multi-index

**Additional Inherited Members**

13.120.1 Detailed Description

Derived nondeterministic class that generates N-dimensional numerical quadrature points for evaluation of expectation integrals over uncorrelated standard normals/uniforms/exponentials/betas/gammas.

This class is used by `NonDPolynomialChaos`, but could also be used for general numerical integration of moments. It employs Gauss-Hermite, Gauss-Legendre, Gauss-Laguerre, Gauss-Jacobi and generalized Gauss-Laguerre quadrature for use with normal, uniform, exponential, beta, and gamma density functions and integration bounds. The abscissas and weights for one-dimensional integration are extracted from the appropriate Orthogonal-Polynomial class and are extended to n-dimensions using a tensor product approach.

13.120.2 Constructor & Destructor Documentation

`NonDQuadrature ( Model & model, const UShortArray & quad_order_seq, const RealVector & dim_pref, short driver_mode )`

alternate constructor for instantiations "on the fly" based on a quadrature order specification

This alternate constructor is used for on-the-fly generation and evaluation of numerical quadrature points. References `NonDIntegration::numIntDriver`, and `NonDQuadrature::tpqDriver`. 

References NonDIntegration::numIntDriver, and NonDQuadrature::tpqDriver.
NonDQuadrature ( Model & model, int num_filt_samples, const RealVector & dim_pref, short driver_mode )

alternate constructor for instantiations "on the fly" that generate a filtered tensor product sample set

This alternate constructor is used for on-the-fly generation and evaluation of filtered tensor quadrature points.

References NonDIntegration::numIntDriver, and NonDQuadrature::tpqDriver.

NonDQuadrature ( Model & model, int num_rand_samples, int seed, const UShortArray & quad_order_seq, const RealVector & dim_pref, short driver_mode )

alternate constructor for instantiations "on the fly" that sample randomly from a tensor product multi-index

This alternate constructor is used for on-the-fly generation and evaluation of random sampling from a tensor quadrature multi-index.

References NonDIntegration::numIntDriver, and NonDQuadrature::tpqDriver.

NonDQuadrature ( ProblemDescDB & problem_db, Model & model ) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. It is not currently used, as there is not yet a separate nond_quadrequation method specification.

References NonDIntegration::check_variables(), Iterator::convergenceTol, ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_short(), ProblemDescDB::get_ushort(), Iterator::maxEvalConcurrency, NonD::natafTransform, NonDQuadrature::nestedRules, NonIntegration::numIntDriver, Iterator::outputLevel, Iterator::probDescDB, NonDQuadrature::reset(), and NonDQuadrature::tpqDriver.

13.120.3 Member Function Documentation

void initialize_grid ( const std::vector< Pecos::BasisPolynomial > & poly_basis ) [protected], [virtual]

Used in combination with alternate NonDQuadrature constructor.

Implements NonDIntegration.

References Iterator::maxEvalConcurrency, NonDQuadrature::nestedRules, Analyzer::numContinuousVars, NonDQuadrature::numSamples, NonDQuadrature::quadMode, NonDQuadrature::reset(), NonDQuadrature::tpqDriver, and NonDQuadrature::update().

void sampling_reset ( int min_samples, bool all_data_flag, bool stats_flag ) [protected], [virtual]

used by DataFitSurrModel::build_global() to publish the minimum number of points needed from the quadrature routine in order to build a particular global approximation.

Reimplemented from Iterator.

References NonDQuadrature::compute_minimum_quadrature_order(), NonDIntegration::dimPrefSpec, NonDQuadrature::dimQuadOrderRef, NonDQuadrature::nestedRules, Analyzer::numContinuousVars, and NonDQuadrature::tpqDriver.

Referenced by NonDQuadrature::update().

int num_samples ( ) const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.
Reimplemented from Analyzer.
References NonDQuadrature::numSamples, NonDQuadrature::quadMode, and NonDQuadrature::tpqDriver.
The documentation for this class was generated from the following files:

- NonDQuadrature.hpp
- NonDQuadrature.cpp

13.121  NonDQUESOBayesCalibration Class Reference

Bayesian inference using the QUESO library from UT Austin.

Inheritance diagram for NonDQUESOBayesCalibration:

```
  Iterator
    Analyzer
      NonD
        NonDCalibration
          NonDBayesCalibration
            NonDQUESOBayesCalibration
```

Public Member Functions

- **NonDQUESOBayesCalibration** (ProblemDescDB &problem_db, Model &model)
  _standard constructor_

- ~**NonDQUESOBayesCalibration** ()
  _destructor_

Protected Member Functions

- void **calibrate** ()
- void **print_results** (std::ostream &s)
  _print the final iterator results_
- void **init_queso_environment** (const String &input_filename=String())
  _initialize the QUESO FullEnvironment on the Dakota MPIComm_
- void **init_precond_request_value** ()
  _initialize the ASV value for preconditioned cases_
- virtual void **init_queso_solver** ()
define solver options, likelihood callback, posterior RV, and inverse problem

- void precondition_proposal()
  use derivative information from the emulator to define the proposal covariance (inverse of misfit Hessian)
- void run_queso_solver()
  perform the MCMC process
- void run_chain_with_restarting()
  short term option to restart the MCMC chain with updated proposal density computed from the emulator at a new starting point
- void accumulate_chain(size_t update_cntr)
  accumulate unique samples drawn from the acceptance chain
- void aggregate_acceptance_chain(size_t update_cntr)
  accumulate the acceptance chain across multiple restart cycles, including recovering corresponding function values
- void filter_chain_by_probability(size_t update_cntr, unsigned short batch_size)
  extract batch size points from the MCMC chain and store final aggregated set within allSamples; unique points with highest posterior probability are selected
- void filter_chain_by_conditioning(size_t update_cntr, unsigned short batch_size)
  extract batch size points from the MCMC chain and store final aggregated set within allSamples; unique points with best conditioning are selected, as determined by pivoted LU
- void chain_to_local(unsigned short batch_size, std::map<Real, size_t>&local_best)
  store indices of best batch size samples from the current MCMC chain within the local_best array
- void local_to_aggregated(unsigned short batch_size, const std::map<Real, size_t>&local_best)
  update bestSamples aggregation using new contributions from the current MCMC chain
- void aggregated_to_all()
  following aggregation cycles, copy bestSamples to allSamples
- void local_to_all(const std::map<Real, size_t>&local_best)
  in the absence of aggregation cycles, copy local_best to allSamples
- void update_center()
  update the starting point for a restarted MCMC chain using last point from previous chain
- void update_model()
  evaluates allSamples on iteratedModel and update the mcmcModel emulator with all\{Samples,Responses\}
- Real assess_emulator_convergence()
  compute the L2 norm of the change in emulator coefficients
- void init_parameter_domain()
  initialize the QUESO parameter space, min, max, initial, and domain
- void init_proposal_covariance()
- void prior_proposal_covariance()
  use covariance of prior distribution for setting proposal covariance
- void user_proposal_covariance(const String &input_fmt, const RealVector &cov_data, const String &cov_-filename)
  set proposal covariance from user-provided diagonal or matrix
- void validate_proposal()
- void set_ip_options()
  set inverse problem options callIpOptionsValues common to all solvers
- void set_mh_options()
13.121. NONDQESOBAYESCALIBRATION CLASS REFERENCE

```cpp
set MH-specific inverse problem options callIpMhOptionsValues
• void update_chain_size (unsigned int size)
  update MH-specific inverse problem options callIpMhOptionsValues
• void copy_gsl (const QUESO::GslVector &qv, RealVector &rv)
  local copy data utility from GslVector to RealVector
• void copy_gsl (const RealVector &rv, QUESO::GslVector &qv)
  local copy data utility from RealVector to GslVector
• void copy_gsl_partial (const QUESO::GslVector &qv, size_t start, RealVector &rv)
  local copy data utility from portion of GslVector to RealVector
• void copy_gsl_partial (const RealVector &rv, QUESO::GslVector &qv, size_t start)
  local copy data utility from RealVector to portion of GslVector
• void copy_gsl (const QUESO::GslVector &qv, RealMatrix &rm, int i)
  local copy data utility from GslVector to column in RealMatrix
• bool equal_gsl (const QUESO::GslVector &qv1, const QUESO::GslVector &qv2)
  equality tester for two GslVectors
```

Static Protected Member Functions

```cpp
• static double dakotaLogLikelihood (const QUESO::GslVector &paramValues, const QUESO::GslVector *paramDirection, const void *functionDataPtr, QUESO::GslVector *gradVector, QUESO::GslMatrix *hessianMatrix, QUESO::GslVector *hessianEffect)
  Log Likelihood function for call-back from QUESO to DAKOTA for evaluation.
```

Protected Attributes

```cpp
• String mcmcType
  MCMC type ("dram" or "delayed_rejection" or "adaptive_metropolis" or "metropolis_hastings" or "multilevel", within QUESO)
• short precondRequestValue
  the active set request value to use in proposal preconditioning
• bool logitTransform
  flag indicating user activation of logit transform option
• boost::shared_ptr < QUESO::EnvOptionsValues > envOptionsValues
  options for setting up the QUESO Environment
• boost::shared_ptr < QUESO::FullEnvironment > quesoEnv
  top-level QUESO Environment
• boost::shared_ptr < QUESO::VectorSpace >
  < QUESO::GslVector, QUESO::GslMatrix > > paramSpace
  QUESO parameter space based on number of calibrated parameters.
```
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- boost::shared_ptr
  < QUESO::BoxSubset
  < QUESO::GslVector,
  QUESO::GslMatrix > > paramDomain
  QUESO parameter domain: hypercube based on min/max values.

- boost::shared_ptr
  < QUESO::GslVector > paramInitials
  initial parameter values at which to start chain

- boost::shared_ptr
  < QUESO::BaseVectorRV
  < QUESO::GslVector,
  QUESO::GslMatrix > > priorRv

- boost::shared_ptr
  < QUESO::GslMatrix > proposalCovMatrix
  proposal covariance for DRAM

- boost::shared_ptr
  < QUESO::SipOptionsValues > calIpOptionsValues
  general inverse problem options

- boost::shared_ptr
  < QUESO::MhOptionsValues > calIpMhOptionsValues
  MH-specific inverse problem options.

- boost::shared_ptr
  < QUESO::GenericScalarFunction
  < QUESO::GslVector,
  QUESO::GslMatrix > > likelihoodFunctionObj

- boost::shared_ptr
  < QUESO::GenericVectorRV
  < QUESO::GslVector,
  QUESO::GslMatrix > > postRv

- boost::shared_ptr
  < QUESO::StatisticalInverseProblem
  < QUESO::GslVector,
  QUESO::GslMatrix > > inverseProb

Static Protected Attributes
- static NonDQUESOBayesCalibration * nonDQUESOInstance
  Pointer to current class instance for use in static callback functions.

Private Attributes
- RealVectorArray uniqueSamples
  container for aggregating unique MCMC sample points collected across multiple (restarted) chains

- RealVectorArray prevCoeffs
  cache previous expansion coefficients for assessing convergence of emulator refinement process

- RealVector mapSoln
  store MAP estimate for warm-starting pre-solves
13.121. NONDQUESOBAYESCALIBRATION CLASS REFERENCE

Additional Inherited Members

13.121.1 Detailed Description

Bayesian inference using the QUESO library from UT Austin.

This class provides a wrapper to the QUESO library developed as part of the Predictive Science Academic
Alliance Program (PSAAP), specifically the PECOS (Predictive Engineering and Computational Sciences) Cen-
ter at UT Austin. The name QUESO stands for Quantification of Uncertainty for Estimation, Simulation, and
Optimization.

13.121.2 Constructor & Destructor Documentation

NonDQUESOBayesCalibration ( ProblemDescDB & problem_db, Model & model )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes
has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDCalibration::calibrationData, NonDQUESOBayesCalibration::init-
queso_environment(), and NonDBayesCalibration::obsErrorMultiplierMode.

13.121.3 Member Function Documentation

void calibrate ( ) [protected], [virtual]

Perform the uncertainty quantification

Implements NonDBayesCalibration.

References Dakota::abort_handler(), NonDBayesCalibration::adaptPosteriorRefine, NonDQUESOBayesCalibration-
::assess_emulator_convergence(), Analyzer::compactMode, NonDBayesCalibration::compute_statistics(), Iterator-
::convergenceTol, NonDBayesCalibration::emulatorType, NonDQUESOBayesCalibration::init_parameter_domain(),
NonDQUESOBayesCalibration::init_precond_request_value(), NonDQUESOBayesCalibration::init_queso_solver(),
NonDBayesCalibration::initialize_model(), Iterator::maxIterations, NonDQUESOBayesCalibration::nonDQUE-
SOInstance, NonDQUESOBayesCalibration::precondRequestValue, NonDBayesCalibration::proposalCovarType,
NonDQUESOBayesCalibration::run_chain_with_restarting(), and NonDQUESOBayesCalibration::update_model().

void print_results ( std::ostream & s ) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation
summary printed in finalize_run().

Reimplemented from NonDBayesCalibration.

References NonDBayesCalibration::bestSamples, Model::continuous_variable_labels(), Dakota::copy_data(),
NonDQUESOBayesCalibration::copy_gsl(), NonDQUESOBayesCalibration::copy_gsl_partial(), NonDCalibration-
::expData, Dakota::HALF_LOG_2PI, ExperimentData::half_log_cov_determinant(), Iterator::iteratedModel, Non-
DBayesCalibration::log_prior_density(), NonD::natafTransform, Model::num_primary_fns(), Analyzer::numContinuous-
Vars, NonDBayesCalibration::numHyperparams, NonDBayesCalibration::obsErrorMultiplierMode, NonDQUE-
SOBayesCalibration::paramSpace, NonDBayesCalibration::print_results(), NonDBayesCalibration::residualModel,
NonDBayesCalibration::standardizedSpace, and Dakota::write_precision.

void init_queso_environment ( const String & input_filename = String() ) [protected]

initialize the QUESO FullEnvironment on the Dakota MPIComm
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The input filename is only passed by GPMSA as there’s no way to override the C++ options with file-based options for the QUESO ctors.

References NonDQUESOBayesCalibration::envOptionsValues, NonDQUESOBayesCalibration::mcmcType, ParallelLibrary::mpirun_flag(), Iterator::parallelLib, NonDQUESOBayesCalibration::quesoEnv, and NonDBayesCalibration::randomSeed.

Referenced by NonDGPMSSABayesCalibration::NonDGPMSSABayesCalibration(), and NonDQUESOBayesCalibration::NonDQUESOBayesCalibration().

```cpp
void aggregate_acceptance_chain ( size_t cycle_num ) [protected]
accumulate the acceptance chain across multiple restart cycles, including recovering corresponding function values

Populate a subset of acceptanceChain(num_params, chainSamples * chainCycles) and acceptedFnVals(numFunctions, chainSamples * chainCycles)

References NonDBayesCalibration::acceptanceChain, NonDBayesCalibration::acceptedFnVals, Response::active_set(), Model::active_variables(), NonDBayesCalibration::chainSamples, Variables::continuous_variables(), Response::copy(), Variables::copy(), NonDQUESOBayesCalibration::copy_gsl_partial(), Model::current_response(), Model::current_variables(), Dakota::data_pairs, Model::evaluate(), Response::function_values(), Model::interface_id(), Dakota::lookup_by_val(), NonDBayesCalibration::mcmcModel, NonDBayesCalibration::mcmcModelHasSurrogate, Model::model_type(), NonD::natafTransform, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, ActiveSet::request_values(), NonDBayesCalibration::standardizedSpace, and ParamResponsePair::variables().

Referenced by NonDQUESOBayesCalibration::run_chain_with_restarting().
```

```cpp
void init_parameter_domain ( ) [protected]
initialize the QUESO parameter space, min, max, initial, and domain

Initialize the calibration parameter domain (paramSpace, paramMins/paramMaxs, paramDomain, paramInitials, priorRV)

References Model::continuous_variables(), NonDQUESOBayesCalibration::copy_gsl_partial(), NonDBayesCalibration::emulatorType, NonDBayesCalibration::invGammaDists, NonDBayesCalibration::mcmcModel, NonD::natafTransform, NonDQUESOBayesCalibration::nonDQUESOInstance, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, NonDQUESOBayesCalibration::paramDomain, NonDQUESOBayesCalibration::paramInitials, NonDQUESOBayesCalibration::paramSpace, NonDQUESOBayesCalibration::quesoEnv, and NonDBayesCalibration::standardizedSpace.

Referenced by NonDQUESOBayesCalibration::calibrate(), and NonDGPMSSABayesCalibration::calibrate().
```

```cpp
void prior_proposal_covariance ( ) [protected]
use covariance of prior distribution for setting proposal covariance

Must be called after paramMins/paramMaxs set above

References NonD::natafTransform, Analyzer::numContinuousVars, Iterator::outputLevel, NonDQUESOBayesCalibration::proposalCovMatrix, and NonDBayesCalibration::standardizedSpace.
```

```cpp
void user_proposal_covariance ( const String & input_fmt, const RealVector & cov_data, const String & cov_filename ) [protected]
set proposal covariance from user-provided diagonal or matrix

This function will convert user-specified cov_type = "diagonal" | "matrix" data from either cov_data or cov_filename and populate a full QUESO::GslMatrix* in proposalCovMatrix with the covariance.
```
References Analyzer::numContinuousVars, NonDQUESOBayesCalibration::proposalCovMatrix, and NonDBayesCalibration::standardizedSpace.

```cpp
void set_ip_options() [protected]
```

set inverse problem options callIpOptionsValues common to all solvers

set inverse problem options common to all solvers

References NonDQUESOBayesCalibration::callIpOptionsValues.

Referenced by NonDQUESOBayesCalibration::init_queso_solver(), and NonDGPMSABayesCalibration::init_queso_solver().

### 13.121.4 Member Data Documentation

```cpp
bool logitTransform [protected]
```

flag indicating user activation of logit transform option

this option is useful for preventing rejection or resampling for out-of-bounds samples by transforming bounded domains to [-inf,inf].

Referenced by NonDQUESOBayesCalibration::set_mh_options().

The documentation for this class was generated from the following files:

- NonDQUESOBayesCalibration.hpp
- NonDQUESOBayesCalibration.cpp

### 13.122 NonDReliability Class Reference

Base class for the reliability methods within DAKOTA/UQ.

Inheritance diagram for NonDReliability:

```
NonDGlobalReliability
NonDLocalReliability
NonD
NonDReliability
Analyzer
Iterator
```

#### Public Member Functions

- `bool resize()`  
  
  reinitializes iterator based on new variable size
Protected Member Functions

- **NonDReliability** (ProblemDescDB &problem_db, Model &model)
  constructor

- **~NonDReliability ()**
  destructor

- **void initialize_graphics (int iterator_server_id=1)**
  initialize graphics customized for reliability methods

- **const Model & algorithm_space_model () const**

Protected Attributes

- **Model uSpaceModel**
  Model representing the limit state in u-space, after any recastings and data fits.

- **Model mppModel**
  RecastModel which formulates the optimization subproblem: RIA, PMA, EGO.

- **Iterator mppOptimizer**
  Iterator which optimizes the mppModel.

- **unsigned short mppSearchType**
  the MPP search type selection: MV, x/u-space AMV, x/u-space AMV+, x/u-space TANA, x/u-space EGO, or NO_A-PROM

- **Iterator importanceSampler**
  importance sampling instance used to compute/refine probabilities

- **unsigned short integrationRefinement**
  integration refinement type (NO_INT_REFINE, IS, AIS, or MMAIS) provided by refinement specification

- **size_t numRelAnalyses**
  number of invocations of core_run()

- **size_t approxIters**
  number of approximation cycles for the current respFnCount/levelCount

- **bool approxConverged**
  indicates convergence of approximation-based iterations

- **int respFnCount**
  counter for which response function is being analyzed

- **size_t levelCount**
  counter for which response/probability level is being analyzed

- **size_t statCount**
  counter for which final statistic is being computed

- **bool pmaMaximizeG**
  flag indicating maximization of G(u) within PMA formulation

- **Real requestedTargetLevel**
  the {response, reliability, generalized reliability} level target for the current response function
Additional Inherited Members

13.122.1 Detailed Description

Base class for the reliability methods within DAKOTA/UQ.

The NonDReliability class provides a base class for NonDLocalReliability, which implements traditional MPP-based reliability methods, and NonDGlobalReliability, which implements global limit state search using Gaussian process models in combination with multimodal importance sampling.

13.122.2 Member Function Documentation

const Model & algorithm_space_model( ) const [inline],[protected],[virtual]

default definition that gets redefined in selected derived Minimizers
Reimplemented from Analyzer.
References NonDReliability::uSpaceModel.
The documentation for this class was generated from the following files:

- NonDReliability.hpp
- NonDReliability.cpp

13.123 NonDRKDDarts Class Reference

Base class for the Recursive k-d Dart methods within DAKOTA/UQ.

Inheritance diagram for NonDRKDDarts:

```
    Iterator
     |
     v
    Analyzer
         |
         v
        NonD
            |
            v
            NonDRKDDarts
```

Public Member Functions

- **NonDRKDDarts** (ProblemDescDB &problem_db, Model &model)
  *constructor*

- **~NonDRKDDarts** ()
  *destructor*

- **bool resize ()**
  *reinitializes iterator based on new variable size*

- **void core_run ()**
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Protected Member Functions

- void pre_run ()
  
  generate samples

- void initiate_random_number_generator (unsigned long x)

- double generate_a_random_number ()

- void init_rkd_darts ()

- void create_rkd_containers (size_t expected_num_samples)

- void execute ()

- void create_initial_children (size_t parent)

- void create_new_sample (size_t parent, size_t left, size_t right, double position)

- void improve_parent_evaluation (size_t parent)

- void evaluate_1d_surrogate (size_t parent)

- double get_surrogate_interp_error (size_t parent)

- double estimate_surrogate_evaluation_err (size_t parent)

- void get_children (size_t parent, size_t *children)

- void get_neighbors (size_t sample, size_t &num_neighbors, size_t *neighbors)

- double interpolate_lagrange (size_t num_data_points, double *data_x, double *data_f, double x)

- double integrate_legendre_gauss (double xmin, double xmax, size_t num_data_points, double *data_x, double *data_f, double &err_est)

- double f_true (double *x)

- void initialize_surrogates ()

- void compute_response (double *x)

- void add_surrogate_data (const Variables &vars, const Response &resp)

- void build_surrogate ()

- double eval_surrogate (size_t fn_index, double *vin)

- void estimate_rkd_surrogate ()

- void post_run (std::ostream &s)

- void print_integration_results (std::ostream &s)

- void exit_rkd_darts ()

- void destroy_rkd_containers ()

Protected Attributes

- int samples

- int seed

- int emulatorSamples

- double Q [1220]

- int index

- double cc

- double c

- double ze

- double zx

- double zy

- size_t qlen
Private Attributes

- double * _I_RKD
- bool _eval_error
- size_t _test_function
- size_t _num_inserted_points
- size_t _num_dim
- size_t _num_samples
- size_t _max_num_samples
- size_t _num_evaluations
- size_t _evaluation_budget
- size_t _max_num_neighbors
- double _bounding_box_volume
- double _discont_jump_threshold
- double * _xmin
- double * _xmax
- double ** fval
- size_t * _sample_dim
- size_t * _sample_parent
- size_t * _sample_first_child
- size_t * _sample_num_children
- size_t * _sample_left
- size_t * _sample_right
- double * _sample_coord
- double * _sample_value
- double * _sample_left_interp_err
- double * _sample_right_interp_err
- double * _sample_left_ev_err
- double * _sample_right_ev_err

Additional Inherited Members

13.123.1 Detailed Description

Base class for the Recursive k-d Dart methods within DAKOTA/UQ.

The NonDRKDDart class recursively implements the numerical integration of a domain based on k-d flat samples.

13.123.2 Member Function Documentation

void core_run() [virtual]

Loop over the set of samples and compute responses.
Reimplemented from Iterator.

void pre_run() [protected], [virtual]

generate samples
Generate Parameter Sets.
Reimplemented from Analyzer.
References Analyzer::pre_run().
void post_run ( std::ostream &s ) [protected], [virtual]

generate statistics
Print function evaluation summary, and integration results.
Reimplemented from Analyzer.
References Iterator::iteratedModel, Analyzer::post_run(), and Model::print_evaluation_summary().
The documentation for this class was generated from the following files:

- NonDRKDDarts.hpp
- NonDRKDDarts.cpp

### 13.124 NonDSampling Class Reference

Base class for common code between NonDLHSSampling, NonDAdaptImpSampling, and other specializations.

Inheritance diagram for NonDSampling:

```
      iterator
     /     \
    /       \
  analyzer
     |       |
    |       |  nonD
    |       |
  nonDSampling
    |       |
  NonDAdaptImpSampling NonDAdaptiveSampling NonDGPImpSampling NonDLHSSampling NonDMultilevelSampling
```

#### Public Member Functions

- **NonDSampling** (Model &model, const RealMatrix &sample_matrix)
  
  alternate constructor for evaluating and computing statistics for the provided set of samples
- **void compute_statistics** (const RealMatrix &vars_samples, const IntResponseMap &resp_samples)
  
  For the input sample set, computes mean, standard deviation, and probability/reliability/response levels (aleatory uncertainties) or intervals (epistemic or mixed uncertainties)
- **void compute_intervals** (RealRealPairArray &extreme_fns)
  
  called by compute_statistics() to calculate min/max intervals using allResponses
- **void compute_intervalls** (const IntResponseMap &samples)
  
  called by compute_statistics() to calculate extremeValues from samples
- **void compute_intervals** (RealRealPairArray &extreme_fns, const IntResponseMap &samples)
  
  called by compute_statistics() to calculate min/max intervals using samples
- **void compute_moments** (const RealMatrix &samples)
  
  calculates sample moments from a matrix of observations for a set of QoI
- **void compute_moments** (const IntResponseMap &samples)
  
  calculate sample moments and confidence intervals from a map of response observations
- **void compute_moments** (const IntResponseMap &samples, RealMatrix &moment_stats, RealMatrix &moment_conf ints, short moments_type, const StringArray &labels)
  
  convert IntResponseMap to RealMatrix and invoke helpers
- **void archive_moments** (const RealMatrix &moment_stats, short moments_type, const StringArray &labels)
archive moment statistics in results DB

- void archive_moment_confidence_intervals (const RealMatrix &moment_conf_ints, short moments_type, const StringArray &labels)

archive moment confidence intervals in results DB

- void compute_level_mappings (const IntResponseMap &samples)

called by compute_statistics() to calculate CDF/CCDF mappings of z to p/beta and of p/beta to z as well as PDFs

- void print_statistics (std::ostream &s) const

prints the statistics computed in compute_statistics()

- void print_intervals (std::ostream &s) const

prints the intervals computed in compute_intervals() with default qoi_type and moment_labels

- void print_intervals (std::ostream &s, String qoi_type, const StringArray &interval_labels) const

prints the intervals computed in compute_intervals()

- void print_moments (std::ostream &s) const

prints the moments computed in compute_moments() with default qoi_type and moment_labels

- void print_moments (std::ostream &s, String qoi_type, const StringArray &moment_labels) const

prints the moments computed in compute_moments()

- void print_wilks_statistics (std::ostream &s) const

prints the Wilks statistics

- void update_final_statistics ()

update finalStatistics from minValues/maxValues, finalMomentStats, and computedProbLevels/computedRelLevels/computed-RespLevels

- void transform_samples (bool x_to_u=true)

transform allSamples imported by alternate constructor. This is needed since random variable distribution parameters are not updated until run time and an imported sample_matrix is typically in x-space.

- void transform_samples (RealMatrix &sample_matrix, bool x_to_u, int num_samples=0)

transform the specified samples matrix from x to u or u to x

Static Public Member Functions

- static void compute_moments (const RealMatrix &samples, SizetArray &sample_counts, RealMatrix &moment_stats, short moments_type, const StringArray &labels)

core compute_moments() implementation with all data as inputs

- static void compute_moments (const RealMatrix &samples, RealMatrix &moment_stats, short moments_type)

core compute_moments() implementation with all data as inputs

- static void compute_moment_confidence_intervals (const RealMatrix &moment_stats, RealMatrix &moment_conf_ints, const SizetArray &sample_counts, short moments_type)

compute moment confidence intervals from moment values

- static void print_moments (std::ostream &s, const RealMatrix &moment_stats, const RealMatrix moment_cis, String qoi_type, short moments_type, const StringArray &moment_labels, bool print_cis)

core print moments that can be called without object

- static int compute_wilks_sample_size (unsigned short order, Real alpha, Real beta, bool twosided=false)

calculates the number of samples using the Wilks formula Static so I can test without instantiating a NonDSampling object - RWH

- static Real compute_wilks_residual (unsigned short order, int nsamples, Real alpha, Real beta, bool twosided)
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Helper function - calculates the Wilks residual.

- static Real compute_wilks_alpha (unsigned short order, int nsamples, Real beta, bool twosided=false) calculates the alpha parameter given number of samples using the Wilks formula Static so I can test without instantiating a NonDSampling object - RWH
- static Real compute_wilks_beta (unsigned short order, int nsamples, Real alpha, bool twosided=false) calculates the beta parameter given number of samples using the Wilks formula Static so I can test without instantiating a NonDSampling object - RWH
- static Real get_wilks_alpha_min ()
  Get the lower and upper bounds supported by Wilks bisection solves.
- static Real get_wilks_alpha_max ()
- static Real get_wilks_beta_min ()
- static Real get_wilks_beta_max ()

Protected Member Functions

- NonDSampling (ProblemDescDB &problem_db, Model &model)
  constructor
- NonDSampling (unsigned short method_name, Model &model, unsigned short sample_type, int samples, int seed, const String &rng, bool vary_pattern, short sampling_vars_mode)
  alternate constructor for sample generation and evaluation "on the fly"
- NonDSampling (unsigned short sample_type, int samples, int seed, const String &rng, const RealVector &lower_bnds, const RealVector &upper_bnds)
  alternate constructor for sample generation "on the fly"
- NonDSampling (unsigned short sample_type, int samples, int seed, const String &rng, const RealVector &means, const RealVector &std_devs, const RealVector &lower_bnds, const RealVector &upper_bnds, RealSymMatrix &correl)
  alternate constructor for sample generation of correlated normals "on the fly"
- ~NonDSampling ()
  destructor
- void core_run ()
- int num_samples () const
- void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)
  resets number of samples and sampling flags
- void sampling_reference (int samples_ref)
  set reference number of samples, which is a lower bound during reset
- unsigned short sampling_scheme () const
  return sampleType
- void vary_pattern (bool pattern_flag)
  set varyPattern
- void get_parameter_sets (Model &model)
  Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model.
- void get_parameter_sets (Model &model, const int num_samples, RealMatrix &design_matrix)
  Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model and populates the specified design matrix.
- void get_parameter_sets (Model &model, const int num_samples, RealMatrix &design_matrix, bool write_msg)
  
  core of get_parameter_sets that accepts message print control
- void get_parameter_sets (const RealVector &lower_bnds, const RealVector &upper_bnds)
  
  Uses lhsDriver to generate a set of uniform samples over lower_bnds/upper_bnds.
- void get_parameter_sets (const RealVector &means, const RealVector &std_devs, const RealVector &lower_bnds, const RealVector &upper_bnds, RealSymMatrix &correl)
  
  Uses lhsDriver to generate a set of normal samples.
- void update_model_from_sample (Model &model, const Real∗sample_vars)
  
  Override default update of continuous vars only.
- void sample_to_variables (const Real∗sample_vars, Variables &vars)
  
  override default mapping of continuous variables only
- void variables_to_sample (const Variables &vars, Real∗sample_vars)
- const RealVector & response_error_estimates () const
  
  return error estimates associated with each of the finalStatistics
- void initialize_lhs (bool write_message, int num_samples)
  
  increments numLHSRuns, sets random seed, and initializes lhsDriver
- void view_design_counts (const Model &model, size_t &num_cdv, size_t &num_ddiv, size_t &num_ddsrv, size_t &num_ddrv) const
  
  compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model
- void view_aleatory_uncertain_counts (const Model &model, size_t &num_cauv, size_t &num_dauiv, size_t &num_dausv, size_t &num_daurv) const
  
  compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model
- void view_epistemic_uncertain_counts (const Model &model, size_t &num_ceuv, size_t &num_deuiv, size_t &num_deusv, size_t &num_deurv) const
  
  compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model
- void view_uncertain_counts (const Model &model, size_t &num_cuv, size_t &num_duiv, size_t &num_dusv, size_t &num_durv) const
  
  compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model
- void view_state_counts (const Model &model, size_t &num_csv, size_t &num_dsv, size_t &num_dsrv) const
  
  compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model
- void mode_counts (const Model &model, size_t &cv_start, size_t &num_cv, size_t &div_start, size_t &num_div, size_t &dsv_start, size_t &num_dsv, size_t &drv_start, size_t &num_drv) const
  
  compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model
Static Protected Member Functions

- static void `accumulate_mean` (const RealMatrix &samples, size_t q, size_t &num_samp, Real &mean)
  helper to accumulate sum of finite samples
- static void `accumulate_moments` (const RealMatrix &samples, size_t q, Real *moments, short moments_-type)
  helper to accumulate higher order sums of finite samples

Protected Attributes

- const int `seedSpec`  
  the user seed specification (default is 0)
- int `randomSeed`  
  the current seed
- const int `samplesSpec`  
  initial specification of number of samples
- int `samplesRef`  
  reference number of samples updated for refinement
- int `numSamples`  
  the current number of samples to evaluate
- String `rngName`  
  name of the random number generator
- unsigned short `sampleType`  
  the sample type: default, random, lhs, < incremental random, or incremental lhs
- bool `wilksFlag`  
  flags use of Wilks formula to calculate num samples
- unsigned short `wilksOrder`  

- Real `wilksAlpha`  
- Real `wilksBeta`  
- short `wilksSidedness`  
- RealVector `finalStatErrors`  
  standard errors (estimator std deviation) for each of the finalStatistics
- int `samplesIncrement`  
  current increment in a sequence of samples
- Pecos::LHSDriver `lhsDriver`  
  the C++ wrapper for the F90 LHS library
- bool `statsFlag`  
  flags computation/output of statistics
- bool `allDataFlag`  
  flags update of allResponses  
  < (allVariables or allSamples already defined)
- short `samplingVarsMode`  
  the sampling mode: ALEATORY_UNCERTAIN{,UNIFORM}, EPISTEMIC_UNCERTAIN{,UNIFORM}, UNCERTAIN{,UNIFORM}, ACTIVE{,UNIFORM}, or ALL{,UNIFORM}. This is a secondary control on top of the variables view that allows sampling over subsets of variables that may differ from the view.
• short sampleRanksMode
  
  mode for input/output of LHS sample ranks: IGNORE_RANKS, GET_RANKS, SET_RANKS, or SET_GET_RANKS

• bool varyPattern
  
  flag for generating a sequence of seed values within multiple get_parameter_sets() calls so that these executions
  (e.g., for SBO/SBNLS) are not repeated, but are still repeatable

• RealMatrix sampleRanks
  
  data structure to hold the sample ranks

• SensAnalysisGlobal nonDSampCorr
  
  initialize statistical post processing

• bool backfillFlag
  
  flags whether to use backfill to enforce uniqueness of discrete LHS samples

• RealRealPairArray extremeValues
  
  Minimum and maximum values of response functions for epistemic calculations (calculated in compute_intervals()).

Private Attributes

• size_t numLHSRuns
  
  counter for number of executions of get_parameter_sets() for this object

• RealMatrix finalMomentCIs
  
  Matrix of confidence internals on moments, with rows for mean_lower, mean_upper, sd_lower, sd_upper (calculated
  in compute_moments())

Additional Inherited Members

13.124.1 Detailed Description

Base class for common code between NonDLHSSampling, NonDAdaptImpSampling, and other specializations.

This base class provides common code for sampling methods which employ the Latin Hypercube Sampling
(LHS) package from Sandia Albuquerque’s Risk and Reliability organization. NonDSampling now exclusively
utilizes the 1998 Fortran 90 LHS version as documented in SAND98-0210, which was converted to a UNIX link
library in

1. The 1970’s vintage LHS (that had been f2c’d and converted to incomplete classes) has been removed.

13.124.2 Constructor & Destructor Documentation

NonDSampling ( Model & model, const RealMatrix & sample_matrix )

alternate constructor for evaluating and computing statistics for the provided set of samples

This alternate constructor defines allSamples from an incoming sample matrix.

References Analyzer::allSamples, Analyzer::compactMode, Iterator::maxEvalConcurrency, NonDSampling::
::numSamples, NonDSampling::samplesRef, NonDSampling::samplesSpec, and Iterator::subIteratorFlag.
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NonDSampling (ProblemDescDB & problem_db, Model & model) [protected]

constructor
This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDSampling::compute_wilks_sample_size(), NonD::epistemicStats, ProblemDescDB::get_real(), ProblemDescDB::get_short(), ProblemDescDB::get_ushort(), NonD::initialize_final_statistics(), Iterator::maxEvalConcurrency, Analyzer::numFunctions, NonDSampling::numSamples, Iterator::probDescDB, NonD::requestedProbLevels, NonDSampling::samplesRef, NonDSampling::sampleType, NonD::totalLevelRequests, and NonDSampling::wilksFlag.

NonDSampling (unsigned short method_name, Model & model, unsigned short sample_type, int samples, int seed, const String & rng, bool vary_pattern, short sampling_vars_mode) [protected]

alternate constructor for sample generation and evaluation “on the fly”

This alternate constructor is used for generation and evaluation of on-the-fly sample sets.

References NonD::epistemicStats, Iterator::maxEvalConcurrency, NonD::numEpistemicUncVars, NonDSampling::numSamples, NonDSampling::sampleType, NonDSampling::samplingVarsMode, and Iterator::subIteratorFlag.

NonDSampling (unsigned short sample_type, int samples, int seed, const String & rng, const RealVector & lower_bnds, const RealVector & upper_bnds) [protected]

alternate constructor for sample generation “on the fly”

This alternate constructor is used by ConcurrentStrategy for generation of uniform, uncorrelated sample sets.

References Iterator::maxEvalConcurrency, NonDSampling::numSamples, NonDSampling::sampleType, and Iterator::subIteratorFlag.

NonDSampling (unsigned short sample_type, int samples, int seed, const String & rng, const RealVector & means, const RealVector & std_devs, const RealVector & lower_bnds, const RealVector & upper_bnds, RealSymMatrix & correl) [protected]

alternate constructor for sample generation of correlated normals “on the fly”

This alternate constructor is used by ConcurrentStrategy for generation of normal, correlated sample sets.

References Iterator::maxEvalConcurrency, NonDSampling::numSamples, NonDSampling::sampleType, and Iterator::subIteratorFlag.

13.124.3 Member Function Documentation

void compute_level_mappings (const IntResponseMap & samples)
called by compute_statistics() to calculate CDF/CCDF mappings of z to p/beta and of p/beta to z as well as PDFs

Computes CDF/CCDF based on sample binning. A PDF is inferred from a CDF/CCDF within compute_densities() after level computation.

References Dakota::abort_handler(), NonD::archive_allocate_mappings(), NonD::archive_from_resp(), NonD::archive_to_resp(), NonD::cdfFlag, NonD::compute_densities(), NonD::computedGenRelLevels, NonD::computedProbLevels, NonD::computedRelLevels, NonD::computedRespLevels, NonD::extremeValues, NonD::finalMomentStats, NonD::initialize_level_mappings(), Iterator::iteratedModel, Analyzer::numFunctions, NonD::pdfOutput, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, and Model::response_labels().

Referenced by NonDExpansion::compute_numerical_statistics(), and NonDSampling::compute_statistics().
void core_run() [protected], [virtual]
Default implementation generates allResponses from either allSamples or allVariables.
  Reimplemented from Iterator.
  References NonDSampling::allDataFlag, Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, and NonDSampling::statsFlag.

int num_samples() const [inline], [protected], [virtual]
Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.
  Reimplemented from Analyzer.
  References NonDSampling::numSamples.
  Referenced by NonDAdaptImpSampling::evaluate_samples(), NonDSampling::get_parameter_sets(), NonDSampling::initialize_lhs(), NonDSampling::print_wilks_statistics(), NonDAdaptImpSampling::select_rep_points(), NonDLHSSampling::store_ranks(), and NonDSampling::transform_samples().

void sampling_reset(int min_samples, bool all_data_flag, bool stats_flag) [inline], [protected], [virtual]
resets number of samples and sampling flags
  used by DataFitSurrModel::build_global() to publish the minimum number of samples needed from the sampling routine (to build a particular global approximation) and to set allDataFlag and statsFlag. In this case, allDataFlag is set to true (vectors of variable and response sets must be returned to build the global approximation) and statsFlag is set to false (statistics computations are not needed).
  Reimplemented from Iterator.
  References NonDSampling::allDataFlag, NonDSampling::numSamples, NonDSampling::samplesIncrement, NonDSampling::samplesRef, and NonDSampling::statsFlag.

void get_parameter_sets(Model & model) [protected], [virtual]
Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model.
  This version of get_parameter_sets() extracts data from the user-defined model in any of the four sampling modes and populates class member allSamples.
  Reimplemented from Analyzer.
  References Analyzer::allSamples, and NonDSampling::numSamples.
  Referenced by NonDLHSSampling::compute_pca(), NonDAdaptImpSampling::core_run(), NonDLHSSampling::d_optimal_parameter_set(), NonDSampling::get_parameter_sets(), NonDLHSSampling::increment_lhs_parameter_set(), NonDLHSSampling::initialize_increment_lhs_set(), NonDMultilevelSampling::increment(), NonDMultilevelSampling::multilevel_control_variate_mc_Qcorr(), NonDMultilevelSampling::multilevel_control_variate_mc_Ycorr(), NonDMultilevelSampling::multilevel_mc_Qsum(), NonDMultilevelSampling::multilevel_mc_Ysum(), NonDLHSSampling::NonDLHSSampling(), NonDLHSSampling::pre_run(), and NonDMultilevelSampling::shared_increment().

void get_parameter_sets(Model & model, const int num_samples, RealMatrix & design_matrix) [protected], [virtual]
Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model and populates the specified design matrix.
  This version of get_parameter_sets() extracts data from the user-defined model in any of the four sampling modes and populates the specified design matrix.
  Reimplemented from Analyzer.
References NonDSampling::get_parameter_sets().

```cpp
void get_parameter_sets ( const RealVector & lower_bnds, const RealVector & upper_bnds )
[protected]
```

Uses lhsDriver to generate a set of uniform samples over lower_bnds/upper_bnds.

This version of `get_parameter_sets()` does not extract data from the user-defined model, but instead relies on the incoming bounded region definition. It only support a UNIFORM sampling mode, where the distinction of ACTIVE_UNIFORM vs. ALL_UNIFORM is handled elsewhere.

References Analyzer::allSamples, NonDSampling::initialize_lhs(), NonDSampling::lhsDriver, and NonDSampling::numSamples.

```cpp
void get_parameter_sets ( const RealVector & means, const RealVector & std_devs, const RealVector & lower_bnds, const RealVector & upper_bnds, RealSymMatrix & correl )
[protected]
```

Uses lhsDriver to generate a set of normal samples.

This version of `get_parameter_sets()` does not extract data from the user-defined model, but instead relies on the incoming definition. It only support the sampling of normal variables.

References Analyzer::allSamples, NonDSampling::initialize_lhs(), NonDSampling::lhsDriver, and NonDSampling::numSamples.

```cpp
void variables_to_sample ( const Variables & vars, Real * sample_vars )
[protected], [virtual]
```

Map the active variables from vars to sample_vars (column in allSamples)

Reimplemented from Analyzer.

References Variables::continuous_variables(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), Model::discrete_set_string_values(), Variables::discrete_string_variables(), Iterator::iteratedModel, Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, Dakota::set_value_to_index(), and Variables::view().

```cpp
void view_design_counts ( const Model & model, size_t & num_cdv, size_t & num_ddiv, size_t & num_ddsv, size_t & num_ddrv ) const
[protected]
```

compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model

This function computes total design variable counts, not active counts, for use in defining offsets and counts within all variables arrays.

References Model::current_variables(), Variables::cv_start(), SharedVariablesData::design_counts(), Variables::div_start(), Variables::drv_start(), Variables::dsv_start(), NonD::numContDesVars, NonD::numIntDesVars, NonD::numRealDesVars, NonD::numStringDesVars, Variables::shared_data(), and Variables::view().

Referenced by NonDSampling::mode_counts().

```cpp
void view_aleatory_uncertain_counts ( const Model & model, size_t & num_cauv, size_t & num_dauiv, size_t & num_dausv, size_t & num_dauvr ) const
[protected]
```

compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model

This function computes total aleatory uncertain variable counts, not active counts, for use in defining offsets and counts within all variables arrays.
References SharedVariablesData::aleatory_uncertain_counts(), Model::current_variables(), NonD::numContAleatUncVars, NonD::numDiscIntAleatUncVars, NonD::numDiscRealAleatUncVars, NonD::numDiscStringAleatUncVars, Variables::shared_data(), and Variables::view().

Referenced by NonDSampling::mode_counts().

void view_epistemic_uncertain_counts ( const Model & model, size_t & num_ceuv, size_t & num_deuiv, size_t & num_deusv, size_t & num_derv ) const  [protected]

compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model

This function computes total epistemic uncertain variable counts, not active counts, for use in defining offsets and counts within all variables arrays.

References Model::current_variables(), SharedVariablesData::epistemic_uncertain_counts(), NonD::numContEpistUncVars, NonD::numDiscIntEpistUncVars, NonD::numDiscRealEpistUncVars, NonD::numDiscStringEpistUncVars, Variables::shared_data(), and Variables::view().

Referenced by NonDSampling::mode_counts().

void view_uncertain_counts ( const Model & model, size_t & num_cuv, size_t & num_duiv, size_t & num_dusv, size_t & num_durv ) const  [protected]

compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model

This function computes total uncertain variable counts, not active counts, for use in defining offsets and counts within all variables arrays.

References Model::current_variables(), Variables::cv(), Variables::div(), Variables::drv(), Variables::dsv(), NonD::numContAleatUncVars, NonD::numContEpistUncVars, NonD::numDiscIntAleatUncVars, NonD::numDiscIntEpistUncVars, NonD::numDiscRealAleatUncVars, NonD::numDiscRealEpistUncVars, NonD::numDiscStringAleatUncVars, NonD::numDiscStringEpistUncVars, Variables::shared_data(), SharedVariablesData::uncertain_counts(), and Variables::view().

Referenced by NonDSampling::mode_counts().

void mode_counts ( const Model & model, size_t & cv_start, size_t & num_cv, size_t & div_start, size_t & num_div, size_t & dsv_start, size_t & num_dsv, size_t & drv_start, size_t & num_drv ) const  [protected]

compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model

This function and its helpers to follow are needed since NonDSampling supports a richer set of sampling modes than just the active variable subset. mode_counts() manages the samplingVarsMode setting, while its helper functions (view_{design,aleatory_uncertain,epistemic_uncertain, uncertain,state}counts) manage the active variables view. Similar to the computation of starts and counts in creating active variable views, the results of this function are starts and counts for use within model.all_*() set/get functions.

References Model::acv(), Model::adiv(), Model::adriv(), Model::adsv(), Model::current_variables(), Variables::cv(), Variables::cv_start(), Variables::div(), Variables::div_start(), Variables::drv(), Variables::drv_start(), Variables::dsv(), Variables::dsv_start(), NonDSampling::samplingVarsMode, NonDSampling::view_aleatory_uncertain_counts(), NonDSampling::view_design_counts(), NonDSampling::view_epistemic_uncertain_counts(), and NonDSampling::view_uncertain_counts().

Referenced by NonDSampling::compute_statistics(), NonDLHSSampling::d_optimal_parameter_set(), NonDSampling::get_parameter_sets(), NonDLHSSampling::post_input(), NonDLHSSampling::pre_run(), NonDSampling::print_statistics(), NonDSampling::sample_to_variables(), and NonDSampling::update_model_from_sample().
The documentation for this class was generated from the following files:

- NonDSampling.hpp
- NonDSampling.cpp

## 13.125 NonDSparseGrid Class Reference

Derived nondeterministic class that generates N-dimensional Smolyak sparse grids for numerical evaluation of expectation integrals over independent standard random variables.

Inheritance diagram for NonDSparseGrid:

```
NonDSparseGrid
  NonDIntegration
    NonD
      Analyzer
        Iterator
```

### Public Member Functions

- **NonDSparseGrid** (Model &model, const UShortArray &ssg_level_seq, const RealVector &dim_pref, short exp_coeffs, sohn_approach, short driver_mode, short growth_rate=Pecos::MODERATE_RESTRICTED_GROWTH, short refine_control=Pecos::NO_CONTROL, bool track_uniq_prod_wts=true, bool track_colloc_indices=true)
- **void increment_grid ()**
  ```
  increment ssgDriver::ssgLevel
  ```
- **void increment_grid_weights (const RealVector &aniso_wts)**
  ```
  update ssgDriver::ssgAnisoLevelWts and increment ssgDriver::ssgLevel based on specified anisotropic weighting
  ```
- **void increment_specification_sequence ()**
  ```
  advance to next level in ssgLevelSeqSpec sequence
  ```
- **const std::set<UShortArray> &active_multi_index () const**
  ```
  returns SparseGridDriver::active_multi_index()
  ```
- **void print_smolyak_multi_index () const**
  ```
  invokes SparseGridDriver::print_smolyak_multi_index()
  ```
- **void initialize_sets ()**
  ```
  invokes SparseGridDriver::initialize_sets()
  ```
- **void update_reference ()**
  ```
  invokes SparseGridDriver::update_reference()
  ```
- **void increment_set (const UShortArray &set)**
  ```
  invokes SparseGridDriver::push_trial_set()
  ```
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- **int increment_size () const**
  invokes SparseGridDriver::unique_trial_points()
- **void restore_set ()**
  invokes SparseGridDriver::restore_set()
- **void evaluate_set ()**
  invokes SparseGridDriver::compute_trial_grid()
- **void decrement_set ()**
  invokes SparseGridDriver::pop_trial_set()
- **void update_sets (const UShortArray &set_star)**
  invokes SparseGridDriver::update_sets()
- **void finalize_sets (bool output_sets, bool converged_within_tol)**
  invokes SparseGridDriver::finalize_sets()
- **void evaluate_grid_increment ()**
  invokes SparseGridDriver::evaluate_grid_increment()
- **int num_samples () const**

**Protected Member Functions**

- **NonDSparseGrid (ProblemDescDB &problem_db, Model &model)**
  constructor
- **~NonDSparseGrid ()**
  destructor
- **void initialize_grid (const std::vector<Pecos::BasisPolynomial> &poly_basis)**
  initialize integration grid by drawing from polynomial basis settings
- **void get_parameter_sets (Model &model)**
  Generate one block of numSamples samples (ndim * num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
- **void reset ()**
  restore initial state for repeated sub-iterator executions
- **void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)**

**Private Attributes**

- **Pecos::SparseGridDriver * ssgDriver**
  convenience pointer to the numIntDriver representation
- **UShortArray ssgLevelSeqSpec**
  the user specification for the Smolyak sparse grid level, defining a sequence of refinement levels.
- **unsigned short ssgLevelRef**
  reference point (e.g., lower bound) for the Smolyak sparse grid level maintained within ssgDriver
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Additional Inherited Members

13.125.1 Detailed Description

Derived nondeterministic class that generates N-dimensional Smolyak sparse grids for numerical evaluation of expectation integrals over independent standard random variables.

This class is used by NonDPolynomialChaos and NonDStochCollocation, but could also be used for general numerical integration of moments. It employs 1-D Clenshaw-Curtis and Gaussian quadrature rules within Smolyak sparse grids.

13.125.2 Constructor & Destructor Documentation

NonDSparseGrid ( Model & model, const UShortArray & ssg_level_seq, const RealVector & dim pref, short exp_coeffs soln approach, short driver mode, short growth rate = Pecos::MODERATE_RESTRICTED_GROWTH, short refine control = Pecos::NO_CONTROL, bool track uniq prod wts = true, bool track colloc indices = true )

This alternate constructor is used for on-the-fly generation and evaluation of sparse grids within PCE and SC.

References NonDIntegration::numIntDriver, and NonDSparseGrid::ssgDriver.

NonDSparseGrid ( ProblemDescDB & problem db, Model & model ) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. It is not currently used, as there is not a separate sparse grid method specification.

References Model::aleatory_distribution_parameters(), NonDIntegration::check_variables(), Iterator::convergence-Tol, NonDIntegration::dimPrefSpec, ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_short(), ProblemDescDB::get_ushort(), NonDSparseGrid::initialize_grid(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, NonD::natafTransform, NonDIntegration::numIntDriver, Iterator::outputLevel, Iterator::probDescDB, NonDSparseGrid::ssgDriver, and NonDSparseGrid::ssgLevelRef.

13.125.3 Member Function Documentation

int num_samples ( ) const [inline], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References NonDSparseGrid::ssgDriver.

void sampling_reset ( int min_samples, bool all data flag, bool stats flag ) [protected], [virtual]

used by DataFitSurrModel::build_global() to publish the minimum number of points needed from the sparse grid routine in order to build a particular global approximation.

Reimplemented from Iterator.

References NonDSparseGrid::ssgDriver, and NonDSparseGrid::ssgLevelRef.

The documentation for this class was generated from the following files:

- NonDSparseGrid.hpp
- NonDSparseGrid.cpp
13.126 NonDStochCollocation Class Reference

Nonintrusive stochastic collocation approaches to uncertainty quantification.

Inheritance diagram for NonDStochCollocation:

```
NonDStochCollocation
  └── NonDExpansions
      └── NonD
          └── Iterator
              └── NonDStochCollocation
```

Public Member Functions

- **NonDStochCollocation** (ProblemDescDB &problem_db, Model &model)
  
  *standard constructor*

- **NonDStochCollocation** (Model &model, short exp_coeffs_approach, const UShortArray &num_int_seq, const RealVector &dim_pref, short u_space_type, bool piecewise_basis, bool use_derivs)

  *alternate constructor*

- **~NonDStochCollocation** ()

  *destructor*

- **bool resize** ()

  *reinitializes iterator based on new variable size*

Protected Member Functions

- void **resolve_inputs** (short &u_space_type, short &data_order)

  *perform error checks and mode overrides*

- void **initialize_u_space_model** ()

  *initialize uSpaceModel polynomial approximations with PCE/SC data*

- void **update_expansion** ()

  *update an expansion; avoids overhead in compute_expansion()*

- Real **compute_covariance_metric** ()

  *compute 2-norm of change in response covariance*

- Real **compute_final_statistics_metric** ()

  *compute 2-norm of change in final statistics*
Additional Inherited Members

13.126.1 Detailed Description

Nonintrusive stochastic collocation approaches to uncertainty quantification.

The NonDStochCollocation class uses a stochastic collocation (SC) approach to approximate the effect of parameter uncertainties on response functions of interest. It utilizes the InterpPolyApproximation class to manage multidimensional Lagrange polynomial interpolants.

13.126.2 Constructor & Destructor Documentation

NonDStochCollocation ( ProblemDescDB & problem_db, Model & model )

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References: Response::active_set(), Model::assign_rep(), NonExpansion::check_dimension_preference(), ParallelLibrary::command_line_check(), NonExpansion::construct_expansion_sampler(), NonExpansion::construct_quad(), NonExpansion::construct_sparse_grid(), Model::current_response(), NonExpansion::expansionBasisType, NonExpansion::expansionCoeffsApproach, ProblemDescDB::get_bool(), ProblemDescDB::get_rv(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::get_usa(), ProblemDescDB::get_ushort(), NonExpansion::initialize(), NonDStochCollocation::initialize_u_space_model(), Iterator::iteratedModel, NonExpansion::nestedRules, NonExpansion::numSamplesOnModel, Iterator::outputLevel, Iterator::parallelLib, NonExpansion::piecewiseBasis, Iterator::probDescDB, NonExpansion::refineControl, ActiveSet::request_values(), NonDStochCollocation::resolve_inputs(), NonD::transform_model(), and NonExpansion::uSpaceModel.

NonDStochCollocation ( Model & model, short exp_coeffs_approach, const UShortArray & num_int_seq, const RealVector & dim_pref, short u_space_type, bool piecewise_basis, bool use_derivs )

alternate constructor

This constructor is used for helper iterator instantiation on the fly.

References: Response::active_set(), Model::assign_rep(), NonExpansion::check_dimension_preference(), NonExpansion::construct_quad(), NonExpansion::construct_sparse_grid(), Model::current_response(), NonExpansion::expansionBasisType, NonExpansion::expansionCoeffsApproach, NonExpansion::initialize(), NonDStochCollocation::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, NonExpansion::piecewiseBasis, ActiveSet::request_values(), NonDStochCollocation::resolve_inputs(), NonD::transform_model(), and NonExpansion::uSpaceModel.

13.126.3 Member Function Documentation

Real compute_covariance_metric ( ) [protected], [virtual]

compute 2-norm of change in response covariance

computes the default refinement metric based on change in respCovariance

Reimplemented from NonExpansion.

References: Model::approximations(), NonExpansion::compute_covariance_metric(), PecosApproximation::delta_covariance(), PecosApproximation::expansion_coefficient_flag(), NonExpansion::expansionBasisType, NonExpansion::initializePtU, NonD::numContDesVars, NonD::numContEpistUncVars, NonD::numContStateVars, Analyzer::numFunctions, NonExpansion::respCovariance, and NonExpansion::uSpaceModel.
Real compute_final_statistics_metric() [protected], [virtual]

compute 2-norm of change in final statistics
computes a "goal-oriented" refinement metric employing finalStatistics
Reimplemented from NonDExpansion.
References Model::approximations(), NonD::cdfFlag, NonDExpansion::compute_final_statistics_metric(), NonDExpansion::compute_statistics(), PecosApproximation::delta_beta(), PecosApproximation::delta_z(), PecosApproximation::expansion_coefficient_flag(), NonDExpansion::expansionBasisType, NonD::finalStatistics, Response::function_values(), NonDExpansion::initialPtU, Response::num_functions(), NonD::numContDesVars, NonD::numContEpistUncVars, NonD::numContStateVars, Analyzer::numFunctions, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, and NonDExpansion::uSpaceModel.
The documentation for this class was generated from the following files:

- NonDStochCollocation.hpp
- NonDStochCollocation.cpp

13.127 NonDWASABIBayesCalibration Class Reference

WASABI - Weighted Adaptive Surrogate Approximations for Bayesian Inference.
Inheritance diagram for NonDWASABIBayesCalibration:

```
NonDWASABIBayesCalibration
    NonDBayesCalibration
    NonDCalibration
    NonD
    Analyzer
    Iterator
```

Public Member Functions

- **NonDWASABIBayesCalibration** (ProblemDescDB &problem_db, Model &model)
  _standard constructor_

- ~**NonDWASABIBayesCalibration** ()
  _destructor_

- void **compute_responses** (RealMatrix &samples, RealMatrix &responses)
Static Public Member Functions

- static void problem_size (int &chain_num, int &cr_num, int &gen_num, int &pair_num, int &par_num)
  
  *initializer for problem size characteristics in WASABI*

- static void problem_value (std::string *chain_filename, std::string *gr_filename, double &gr_threshold, int &jumpstep, double limits[], int par_num, int &printstep, std::string *restart_read_filename, std::string *restart_write_filename)

  *Filename and data initializer for WASABI.*

Protected Member Functions

- void calibrate ()
- void print_results (std::ostream &s)
  
  *print the final iterator results*

- void extract_selected_posterior_samples (const std::vector<int> &points_to_keep, const RealMatrix &samples_for_posterior_eval, const RealVector &posterior_density, RealMatrix &posterior_data) const

  *Extract a subset of samples for posterior eval according to the indices in points_to_keep.*

- void export_posterior_samples_to_file (const std::string filename, const RealMatrix &posterior_data) const

  *Export posterior data to file.*

Protected Attributes

- RealVector dataDistMeans
  
  *The mean of the multivariate Gaussian distribution of the obs. data.*

- RealVector dataDistCovariance
  
  *The covariance of the multivariate Gaussian distribution of the obs. data.*

- std::string dataDistFilename
  
  *The filename of the file containing the data that with density estimator defines the distribution of the obs. data.*

- std::string dataDistCovType
  
  *The type of covariance data provided ("diagonal", "matrix")*

- std::string posteriorSamplesImportFile
  
  *The filename of the import file containing samples at which the posterior will be evaluated.*

- unsigned short posteriorSamplesImportFormat
  
  *Format of imported posterior samples file.*

- std::string exportPosteriorDensityFile
  
  *The filename of the export file containing an arbitrary set of samples and their corresponding density values.*

- std::string exportPosteriorSamplesFile
  
  *The filename of the export file containing samples from the posterior and their corresponding density values.*

- unsigned short exportFileFormat
  
  *Format of imported posterior samples and values file.*

- bool generateRandomPosteriorSamples
  
  *Flag specifying whether to generate random samples from the posterior.*

- bool evaluatePosteriorDensity
  
  *Flag specifying whether to evaluate the posterior density at a set of samples.*

- RealVector paramMins
lower bounds on calibrated parameters
- RealVector paramMaxs

upper bounds on calibrated parameters
- boost::mt19937 mumGenerator

random number engine for sampling the prior

Additional Inherited Members

13.127.1 Detailed Description

WASABI - Weighted Adaptive Surrogate Approximations for Bayesian Inference.
This class performs Bayesian calibration using the WASABI approach

13.127.2 Constructor & Destructor Documentation

NonDWASABIBayesCalibration (ProblemDescDB & problem_db, Model & model)

standard constructor
This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes
has been called and probDescDB can be queried for settings from the method specification.

13.127.3 Member Function Documentation

void calibrate ( ) [protected], [virtual]
Perform the uncertainty quantification
- Implements NonDBayesCalibration.
  References Dakota::abort_handler(), Dakota::copy_data(), NonDBayesCalibration::emulatorType, NonDWASABIBayesCalibration::evaluatePosteriorDensity, NonDWASABIBayesCalibration::export_posterior_samples_to_file(), NonDWASABIBayesCalibration::exportPosteriorDensityFile, NonDWASABIBayesCalibration::exportPosteriorSamplesFile, NonDWASABIBayesCalibration::extract_selected_posterior_samples(), NonD::generate_system_seed(), NonDWASABIBayesCalibration::generateRandomPosteriorSamples, NonDBayesCalibration::initialize_model(), NonD::natafTransform, Analyzer::numContinuousVars, Iterator::outputLevel, NonDWASABIBayesCalibration::paramMaxs, NonDWASABIBayesCalibration::paramMins, NonDWASABIBayesCalibration::posteriorSamplesImportFile, NonDBayesCalibration::prior_density(), NonDBayesCalibration::prior_sample(), NonDBayesCalibration::randomSeed, NonDWASABIBayesCalibration::mumGenerator, and NonDBayesCalibration::standardizedSpace.

void print_results ( std::ostream & s ) [protected], [virtual]
print the final iterator results
This virtual function provides additional iterator-specific final results outputs beyond the function evaluation
summary printed in finalize_run().
  Reimplemented from NonDBayesCalibration.
  References NonDBayesCalibration::print_results().
  The documentation for this class was generated from the following files:
- NonDWASABIBayesCalibration.hpp
- NonDWASABIBayesCalibration.cpp
13.128 NonlinearCGOptimizer Class Reference

Inheritance diagram for NonlinearCGOptimizer:

```
NonlinearCGOptimizer
  |        |
  |        |
  |        |
  |        |
  |  Iterator  |
  |    |
  |    |
  |    |
  |    |
  |    |
  |    |
  |    |
  |    |
  Optimizer
  |
  Minimizer
  |
  Optimizer
```

Public Member Functions

- **NonlinearCGOptimizer (ProblemDescDB &problem_db, Model &model)**
  
  *standard constructor*
- **~NonlinearCGOptimizer ()**
  
  *destructor*
- **Real linesearch_eval (const Real &trial_step, short req_val=1)**
  
  *evaluate the objective function given a particular step size (public for use in boost_ls_eval functor; could use friend)*

Protected Member Functions

- **void core_run ()**
  
  *core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post*

Private Member Functions

- **void parse_options ()**
  
  *constructor helper function to parse misc_options from ProblemDescDB*
- **void compute_direction ()**
  
  *compute next direction via choice of method*
- **bool compute_step ()**
  
  *compute step: fixed, simple decrease, sufficient decrease*
- **void bracket_min (Real &xa, Real &xb, Real &xc, Real &fa, Real &fb, Real &fc)**
  
  *bracket the 1-D minimum in the linesearch*
- **Real brent_minimize (Real a, Real b, Real tol)**
  
  *Perform 1-D minimization for the stepLength using Brent's method.*
Private Attributes

- Real initialStep
  *initial step length*
- Real linesearchTolerance
  *approximate accuracy of absissa in LS*
- unsigned linesearchType
  *type of line search (if any)*
- unsigned maxLinesearchIters
  *maximum evaluations in line search*
- Real relFunctionTol
  *stopping criterion for rel change in fn*
- Real relGradientTol
  *stopping criterion for rel reduction in g*
- bool resetStep
  *whether to reset step with each linesearch*
- unsigned restartIter
  *iter at which to reset to steepest descent*
- unsigned updateType
  *type of CG direction update*
- unsigned iterCurr
  *current iteration number*
- RealVector designVars
  *current decision variables in the major iteration*
- RealVector trialVars
  *decision variables in the linesearch*
- Real functionCurr
  *current function value*
- Real functionPrev
  *previous function value*
- RealVector gradCurr
  *current gradient*
- RealVector gradPrev
  *previous gradient*
- RealVector gradDiff
  *temporary for gradient difference (gradCurr - gradPrev)*
- RealVector searchDirection
  *current aggregate search direction*
- Real stepLength
  *current step length parameter alpha*
- Real gradDotGrad_init
  *initial gradient norm squared*
- Real gradDotGrad_curr
  *gradCurr dot gradCurr*
- Real gradDotGrad_prev
  *gradPrev dot gradPrev*
Additional Inherited Members

13.128.1 Detailed Description

Experimental implementation of nonlinear CG optimization

13.128.2 Member Function Documentation

```cpp
void core_run ( ) [protected], [virtual]
```
core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
Reimplemented from Iterator.
References Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, NonlinearCGOptimizer::
compute_direction(), NonlinearCGOptimizer::compute_step(), Model::continuous_variables(), Iterator::convergence-
Tol, Dakota::copy_data(), Model::current_response(), NonlinearCGOptimizer::designVars, Model::evaluate(), Response::
function_gradient_copy(), Response::function_gradient_view(), Response::function_values(), NonlinearCGOptimizer::
functionCurr, NonlinearCGOptimizer::functionPrev, NonlinearCGOptimizer::gradCurr, NonlinearCGOptimizer::
gradDotGrad_curr, NonlinearCGOptimizer::gradDotGrad_init, NonlinearCGOptimizer::gradDotGrad_prev, Nonlinear-
CGOptimizer::gradPrev, Iterator::iteratedModel, NonlinearCGOptimizer::iterCurr, NonlinearCGOptimizer::linesearch-
Type, Optimizer::localObjectiveRecast, Iterator::maxIterations, Minimizer::numContinuousVars, Iterator::output-
Level, NonlinearCGOptimizer::relFunctionTol, NonlinearCGOptimizer::relGradientTol, ActiveSet::request_values(),
NonlinearCGOptimizer::searchDirection, NonlinearCGOptimizer::stepLength, and NonlinearCGOptimizer::trial-
Vars.

```cpp
Real brent_minimize ( Real a, Real b, Real tol ) [private]
```
Perform 1-D minimization for the stepLength using Brent’s method.
Perform 1-D minimization for the stepLength using Brent’s method. This is a C translation of fmin.f from
Netlib.
References NonlinearCGOptimizer::linesearch_eval(), NonlinearCGOptimizer::maxLinesearchIters, and Iterator::
outputLevel.
Referenced by NonlinearCGOptimizer::compute_step().
The documentation for this class was generated from the following files:

- NonlinearCGOptimizer.hpp
- NonlinearCGOptimizer.cpp

13.129 NOWPACBlackBoxEvaluator Class Reference

Derived class for plugging Dakota evaluations into NOWPAC solver.
Inherits BlackBoxBaseClass.

Public Member Functions

- NOWPACBlackBoxEvaluator (Model &model)
  constructor
- void evaluate (std::vector< double > &x, std::vector< double > &vals, void *param)
- void evaluate (std::vector< double > &x, std::vector< double > &vals, std::vector< double > &noise, void *param)
• void allocate_constraints ()
• int num_ineq_constraints () const
• const SizetList & nonlinear_inequality_mapping_indices () const
• const RealList & nonlinear_inequality_mapping_multipliers () const
• const RealList & nonlinear_inequality_mapping_offsets () const

Private Attributes

• Model iteratedModel
  
  cache a local copy of the Model

• int numNowpacIneqConstr
  
  aggregate unsupported constraint types as nonlinear inequalities

• SizetList nonlinIneqConMappingIndices
  
  a list of indices for referencing the DAKOTA nonlinear inequality constraints used in computing the corresponding NOWPAC constraints.

• RealList nonlinIneqConMappingMultipliers
  
  a list of multipliers for mapping the DAKOTA nonlinear inequality constraints to the corresponding NOWPAC constraints.

• RealList nonlinIneqConMappingOffsets
  
  a list of offsets for mapping the DAKOTA nonlinear inequality constraints to the corresponding NOWPAC constraints.

• SizetList linIneqConMappingIndices
  
  a list of indices for referencing the DAKOTA linear inequality constraints used in computing the corresponding NOWPAC constraints.

• RealList linIneqConMappingMultipliers
  
  a list of multipliers for mapping the DAKOTA linear inequality constraints to the corresponding NOWPAC constraints.

• RealList linIneqConMappingOffsets
  
  a list of offsets for mapping the DAKOTA linear inequality constraints to the corresponding NOWPAC constraints.

13.129.1 Detailed Description

Derived class for plugging Dakota evaluations into NOWPAC solver.

The documentation for this class was generated from the following files:

• NOWPACOptimizer.hpp
• NOWPACOptimizer.cpp

13.130 NOWPACOptimizer Class Reference

Wrapper class for the (S)NOWPAC optimization algorithms from Florian Augustin (MIT)

Inheritance diagram for NOWPACOptimizer:
Public Member Functions

- NOWPACOptimizer (ProblemDescDB &problem_db, Model &model)
  *standard constructor*
- NOWPACOptimizer (Model &model)
  *alternate constructor*
- ~NOWPACOptimizer ()
  *destructor*
- void core_run ()
  *core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post*

Private Member Functions

- void initialize_options ()
  *Shared constructor code.*

Private Attributes

- NOWPAC nowpacSolver
- NOWPACBlackBoxEvaluator nowpacEvaluator

Additional Inherited Members

13.130.1 Detailed Description

Wrapper class for the (S)NOWPAC optimization algorithms from Florian Augustin (MIT)

13.130.2 Member Function Documentation

void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Iterator::bestResponseArray, Iterator::bestVariablesArray, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Dakota::copy_data(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, Minimizer::numContinuousVars, Minimizer::numFunctions, Iterator::outputLevel, and Model::primary_response_fn_sense().
The documentation for this class was generated from the following files:

- NOWPACOptimizer.hpp
- NOWPACOptimizer.cpp

### 13.131 NPSOLOptimizer Class Reference

Wrapper class for the NPSOL optimization library.

Inheritance diagram for NPSOLOptimizer:

```
NPSOLOptimizer
  ↓
Minimizer
  ↓
Optimizer
  ↓
SOLBase
```

#### Public Member Functions

- **NPSOLOptimizer** (ProblemDescDB &problem_db, Model &model)
  *standard constructor*

- **NPSOLOptimizer** (Model &model)
  *alternate constructor for Iterator instantiations by name*

- **NPSOLOptimizer** (Model &model, const int &derivative_level, const Real &conv_tol)
  *alternate constructor for instantiations “on the fly”*

  *alternate constructor for instantiations “on the fly”*

- **~NPSOLOptimizer** ()
  *destructor*

- **void core_run** ()
  *core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post*

#### Private Member Functions

- **void find_optimum_on_model** ()
  *called by core_run for setUpType == "model”*

- **void find_optimum_on_user_functions** ()
  *called by core_run for setUpType == "user_functions”*
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Static Private Member Functions

- static void objective_eval (int &mode, int &n, double *x, double &f, double *gradf, int &nstate)

  OBJFUN in NPSOL manual: computes the value and first derivatives of the objective function (passed by function pointer to NPSOL).

Private Attributes

- String setUpType

  controls iteration mode: "model" (normal usage) or "user functions" (user-supplied functions mode for "on the fly" instantiations). NonDReliability currently uses the user functions mode.

- RealVector initialPoint

  holds initial point passed in for "user functions" mode.

- RealVector lowerBounds

  holds variable lower bounds passed in for "user functions" mode.

- RealVector upperBounds

  holds variable upper bounds passed in for "user functions" mode.

- void(* userObjectiveEval )(int &, int &, double *, double &, double *, int &)

  holds function pointer for objective function evaluator passed in for "user functions" mode.

- void(* userConstraintEval )(int &, int &, int &, int &, int *, int *, double *, double *, double *, int &)

  holds function pointer for constraint function evaluator passed in for "user functions" mode.

Static Private Attributes

- static NPSOLOptimizer * npsolInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

13.131.1 Detailed Description

Wrapper class for the NPSOL optimization library.

The NPSOLOptimizer class provides a wrapper for NPSOL, a Fortran 77 sequential quadratic programming library from Stanford University marketed by Stanford Business Associates. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function or accessed through a static pointer.

The user input mappings are as follows: max_function_evaluations is implemented directly in NPSOLOptimizer’s evaluator functions since there is no NPSOL parameter equivalent, and max_iterations, convergence_tolerance, output verbosity, verify_level, function_precision, and linesearch_tolerance are mapped into NPSOL’s "Major Iteration Limit", "Optimality Tolerance", "Major Print Level" (verbose: Major Print Level = 20; quiet: Major Print Level = 10), "Verify Level", "Function Precision", and "Linesearch Tolerance" parameters, respectively, using NPSOL’s npoptn() subroutine (as wrapped by npoptn2() from the npoptn_wrapper.f file). Refer to [Gill, P.E., Murray, W., Saunders, M.A., and Wright, M.H., 1986] for information on NPSOL’s optional input parameters and the npoptn() subroutine.
13.131. NPSOLOPTIMIZER CLASS REFERENCE

13.131.2 Constructor & Destructor Documentation

NPSOLOptimizer ( ProblemDescDB & problem_db, Model & model )

standard constructor

This is the primary constructor. It accepts a Model reference.

References Minimizer::constraintTol, Iterator::convergenceTol, Model::fd_gradient_step_size(), ProblemDesc-
DB::get_int(), ProblemDescDB::get_real(), Model::gradient_type(), Iterator::iteratedModel, Iterator::maxIterations,
Iterator::outputLevel, Iterator::probDescDB, SOLBase::set_options(), Minimizer::speculativeFlag, and Minimizer-::vendorNumericalGradFlag.

NPSOLOptimizer ( Model & model )

alternate constructor for Iterator instantiations by name

This is an alternate constructor which accepts a Model but does not have a supporting method specification
from the ProblemDescDB.

References Minimizer::constraintTol, Iterator::convergenceTol, Model::fd_gradient_step_size(), Model::gradient- _type(), Iterator::iteratedModel, Iterator::maxIterations, Iterator::outputLevel, SOLBase::set_options(), Minimizer-::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

NPSOLOptimizer ( Model & model, const int & derivative_level, const Real & conv_tol )

alternate constructor for instantiations "on the fly"

This is an alternate constructor for instantiations on the fly using a Model but no ProblemDescDB.

NPSOLOptimizer ( const RealVector & initial_point, const RealVector & var_lower_bnds,
const RealVector & var_upper_bnds, const RealMatrix & lin_ineq_coeffs, const RealVector &
lin_ineq_lower_bnds, const RealVector & lin_ineq_upper_bnds, const RealMatrix & lin_eq_coeffs,
const RealVector & lin_eq_targets, const RealVector & nonlin_ineq_lower_bnds, const RealVector &
onlin_ineq_upper_bnds, const RealVector & nonlin_eq_targets, void(*)(int &, int &, double *,
double *, int &) user_obj_eval, void(*)(int &, int &, int &, int &, int, double *, double *,
double *, int &) user_con_eval, const int & derivative_level, const Real & conv_tol )

alternate constructor for instantiations "on the fly"

This is an alternate constructor for performing an optimization using the passed in objective function and
constraint function pointers.

References SOLBase::allocate_arrays(), SOLBase::allocate_workspace(), SOLBase::augment_bounds(), NPSOLOptimizer::lowerBounds, Minimizer::numContinuousVars, Minimizer::numLinearConstraints, Minimizer-::numNonlinearConstraints, and NPSOLOptimizer::upperBounds.

13.131.3 Member Function Documentation

void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Dakota::abort_handler(), NPSOLOptimizer::find_optimum_on_model(), NPSOLOptimizer::find_optimum_on_user_functions(), and NPSOLOptimizer::setUpType.

The documentation for this class was generated from the following files:

- NPSOLOptimizer.hpp
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- NPSOLOptimizer.cpp

13.132 OptDartsOptimizer Class Reference

Wrapper class for OptDarts Optimizer.  
Inheritance diagram for OptDartsOptimizer:

```
Iterator

Minimizer

Optimizer

OptDartsOptimizer
```

Public Member Functions

- OptDartsOptimizer (ProblemDescDB &problem_db, Model &model)  
  Constructor.
- OptDartsOptimizer (Model &model)  
  alternate constructor for Iterator instantiations by name
- ~OptDartsOptimizer ()  
  Destructor.
- void core_run ()  
  Calls the OptDarts algorithm.

Private Member Functions

- void load_parameters (Model &model)  
  Convenience function for Parameter loading.
- double opt_darts_f ()  
  Function evaluation.
- void opt_darts_execute (size_t num_dim, size_t budget, double *xmin, double *xmax, double TOL, size_t problem_index, double fw_MC, double fb_MC)  
  Run the OPT-DARTS method.
- void opt_darts_initiate (double *xmin, double *xmax)  
  Initialize OPT-DARTS.
- void opt_darts_reset_convex_hull ()
- size_t opt_darts_pick_candidate (size_t ifunc)  
  Choose the next trial iterate.
- void retrieve_extended_neighbors (size_t icandidate)
- void opt_darts_sample_from_candidate_neighborhood (size_t icandidate, size_t ifunc)
13.132. **OPTDARTSOPTIMIZER CLASS REFERENCE**

- void **DIRECT_sample_from_candidate_neighborhood** (size_t icandidate)
- void **opt_darts_add_dart** ()
- void **opt_darts_update_K_h_approximate_Voronoi** (size_t isample)
- void **opt_darts_terminate** ()

  *Release memory and exit cleanly.*
- void **opt_darts_plot_discs_2d** (size_t icandidate)

  *Convenience function for plotting iterates.*
- void **opt_darts_plot_hull_2d** (size_t icandidate, size_t ifunc)

  *Convenience function for plotting convex hull.*
- void **initiate_random_generator** (unsigned long x)
- double **generate_a_random_number** ()
- void **sample_uniformly_from_unit_sphere_surface** (double *dart, size_t num_dim)
- bool **trim_line_using_Hyperplane** (size_t num_dim, double *st, double *end, double *qH, double *nH)

**Private Attributes**

- double * _xmin
- double * _xmax
- double * _dart
- double * _st
- double * _end
- double * _tmp_point
- double * _qH
- double * _nH
- double ** _x
- double ** _xc
- double ** _f
- double ** _K
- double * _h
- double * _r
- size_t ** _neighbors
- size_t * _tmp_neighbors
- size_t * _ext_neighbors
- size_t _num_ext_neighbors
- bool _use_opt_darts
- bool _estimate_K
- size_t _ib
- size_t _num_samples
- size_t _budget
- size_t _num_dim
- double _diag
- size_t _problem_index
- double _fb
- double _fw
- double _fval
- size_t _corner_index
• size_t _num_corners
• size_t * _corners
• double _epsilon
• double _fb_MC
• double _fw_MC
• double ** _xm
• double ** _xp
• double * _alpha_Deceptive
• double Q [1220]
• int indx
• double cc
• double c
• double zc
• double zx
• double zy
• size_t qlen
• bool use_DIRECT
• int numTotalVars
• int randomSeed
• int maxBlackBoxEvals
• int maxIterations

Additional Inherited Members

13.132.1 Detailed Description

Wrapper class for OptDarts Optimizer.

The documentation for this class was generated from the following files:

• OptDartsOptimizer.hpp
• OptDartsOptimizer.cpp

13.133 Optimizer Class Reference

Base class for the optimizer branch of the iterator hierarchy.

Inheritance diagram for Optimizer:
### Static Public Member Functions

- `static void not_available (const std::string &package_name)`
  
  *Static helper function: third-party opt packages which are not available.*

### Protected Member Functions

- **Optimizer ()**
  
  *default constructor*

- **Optimizer (ProblemDescDB &problem_db, Model &model)**
  
  *alternate constructor; accepts a model*

- **Optimizer (unsigned short method_name, Model &model)**
  
  *alternate constructor for "on the fly" instantiations*

- **Optimizer (unsigned short method_name, size_t num_cv, size_t num_div, size_t num_dsv, size_t num_drv, size_t num_lin_ineq, size_t num_lin_eq, size_t num_nln_ineq, size_t num_nln_eq)**
  
  *alternate constructor for "on the fly" instantiations*

- **~Optimizer ()**
  
  *destructor*
CHAPTER 13. CLASS DOCUMENTATION

- void initialize_run()
- void post_run(std::ostream &s)
- void finalize_run()

  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- void print_results(std::ostream &s)

Protected Attributes

- size_t numObjectiveFns
  number of objective functions (iterator view)
- bool localObjectiveRecast
  flag indicating whether local recasting to a single objective is used
- Optimizer * prevOptInstance
  pointer containing previous value of optimizerInstance

Static Protected Attributes

- static Optimizer * optimizerInstance
  pointer to Optimizer instance used in static member functions

Private Member Functions

- void reduce_model(bool local_nls_recast, bool require_hessians)
  Wrap iteratedModel in a RecastModel that performs (weighted) multi-objective or sum-of-squared residuals transformation.
- void objective_reduction(const Response &full_response, const BoolDeque &sense, const RealVector &full_wts, Response &reduced_response) const
  forward mapping: maps multiple primary response functions to a single weighted objective for single-objective optimizers

Static Private Member Functions

- static void primary_resp.reducer(const Variables &full_vars, const Variables &reduced_vars, const Response &full_response, Response &reduced_response)
  Recast callback to reduce multiple objectives or residuals to a single objective, with gradients and Hessians as needed.

Additional Inherited Members

13.133.1 Detailed Description

Base class for the optimizer branch of the iterator hierarchy.

The Optimizer class provides common data and functionality for DOTOptimizer, CONMINOptimizer, NPSOLOptimizer, SNLLOptimizer, NLPQLPOptimizer, COLINOptimizer, and JEGAOptimizer.
13.133. **OPTIMIZER CLASS REFERENCE**

### 13.133.2 Member Function Documentation

**void initialize_run**

```
void initialize_run() [protected], [virtual]
```

Implements portions of initialize_run specific to Optimizers. This function should be invoked (or reimplemented) by any derived implementations of initialize_run() (which would otherwise hide it).

- Reimplemented from Minimizer.
- Reimplemented in SNLLOptimizer, NLPQLPOptimizer, and DOTOptimizer.
- References Minimizer::initialize_run(), Iterator::iteratedModel, Iterator::myModelLayers, Optimizer::optimizerInstance, Optimizer::prevOptInstance, and Model::update from subordinate model().
- Referenced by DOTOptimizer::initialize_run(), CONMINOptimizer::initialize_run(), NLPQLPOptimizer::initialize_run(), and SNLLOptimizer::initialize_run().

**void post_run**

```
void post_run(std::ostream & s) [protected], [virtual]
```

Implements portions of post_run specific to Optimizers. This function should be invoked (or reimplemented) by any derived implementations of post_run() (which would otherwise hide it).

- Reimplemented from Minimizer.
- Reimplemented in SNLLOptimizer.
- References Dakota::abort_handler(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Variables::continuous_variables(), ScalingModel::cv_scaled2native(), Minimizer::local_recast_retrieve(), Optimizer::localObjectiveRecast, Model::model_rep(), Minimizer::post_run(), ScalingModel::resp_scaled2native(), Minimizer::scaleFlag, and Minimizer::scalingModel.
- Referenced by COLINOptimizer::post_run(), and SNLLOptimizer::post_run().

**void finalize_run**

```
void finalize_run() [inline], [protected], [virtual]
```

Utility function to perform common operations following post_run(); deallocation and resetting of instance pointers.

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s finalize_run(), typically after performing its own implementation steps.

- Reimplemented from Minimizer.
- Reimplemented in SNLLOptimizer.
- References Minimizer::finalize_run(), Optimizer::optimizerInstance, and Optimizer::prevOptInstance.
- Referenced by SNLLOptimizer::finalize_run().

**void print_results**

```
void print_results(std::ostream & s) [protected], [virtual]
```

Redefines default iterator results printing to include optimization results (objective functions and constraints).

- Reimplemented from Iterator.
- References Dakota::abort_handler(), Minimizer::archive_allocate_best(), Minimizer::archive_best(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, Dakota::data_pairs, Minimizer::dataTransformModel, Model::interface_id(), Dakota::lookup_by_val(), Model::model_rep(), Model::num_functions(), Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, Minimizer::optimizationFlag, Minimizer::original_model(), Model::primary_response_fn_weights(), DataTransformModel::print_best_responses(), and Minimizer::print_residuals().

**void reduce_model**

```
void reduce_model(bool local_tls_recast, bool require_hessians) [private]
```

Wrap iteratedModel in a RecastModel that performs (weighted) multi-objective or sum-of-squared residuals transformation.
Reduce model for least-squares or multi-objective transformation. Doesn’t map variables, or secondary responses. Maps active set for Gauss-Newton. Maps primary responses to single objective so user vs. iterated matters.

References Iterator::activeSet, Model::assign_rep(), Minimizer::calibrationDataFlag, Model::current_response(), Response::function_gradients(), Iterator::gnewton_set_recast(), Model::hessian_type(), Iterator::myModelLayers, Minimizer::numContinuousVars, Minimizer::numFunctions, Minimizer::numIterPrimaryFns, Minimizer::numNonlinearConstraints, Minimizer::numNonlinearIneqConstraints, Optimizer::numObjectiveFns, Minimizer::numTotalCalibTerms, Minimizer::numUserPrimaryFns, Iterator::outputLevel, Model::primary_fn_type(), Optimizer::primary_resp_reducer(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), ActiveSet::request_vector(), and Response::reshape().

Referenced by Optimizer::Optimizer().

```cpp
void primary_resp_reducer ( const Variables & full_vars, const Variables & reduced_vars, const Response & full_response, Response & reduced_response ) [static], [private]
```

Recast callback to reduce multiple objectives or residuals to a single objective, with gradients and Hessians as needed.

Objective function map from multiple primary responses (objective or residuals) to a single objective. Currently supports weighted sum; may later want more general transformations, e.g., goal-oriented

References Iterator::iteratedModel, Optimizer::objective_reduction(), Optimizer::optimizerInstance, Iterator::outputLevel, Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), and Model::subordinate_model().

Referenced by Optimizer::reduce_model().

```cpp
void objective_reduction ( const Response & full_response, const BoolDeque & sense, const RealVector & full_wts, Response & reduced_response ) const [private]
```

forward mapping: maps multiple primary response functions to a single weighted objective for single-objective optimizers

This function is responsible for the mapping of multiple objective functions into a single objective for publishing to single-objective optimizers. Used in DOTOptimizer, NPSOLOptimizer, SNLLOptimizer, and SGOPTAplication on every function evaluation. The simple weighting approach (using primaryRespFnWts) is the only technique supported currently. The weightings are used to scale function values, gradients, and Hessians as needed.

References Response::active_set_request_vector(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian_view(), Response::function_hessians(), Response::function_values(), Response::num_functions(), Minimizer::numConstraints, Minimizer::objective(), Minimizer::objective_gradient(), Minimizer::objective_hessian(), Iterator::outputLevel, and Dakota::write_precision.

Referenced by Optimizer::primary_resp_reducer().

Referenced by Optimizer::reduce_model().

The documentation for this class was generated from the following files:

- DakotaOptimizer.hpp
- DakotaOptimizer.cpp

## 13.134 OutputManager Class Reference

Class to manage redirection of stdout/stderr, keep track of current redir state, and manage rank 0 output. Also manage tabular data output for post-processing with Matlab, Tecplot, etc. and delegate to Graphics for X Windows Graphics.
Public Member Functions

- **OutputManager ()**
  Default constructor (needed for default environment ctors)
- **OutputManager (const ProgramOptions &prog_opts, int dakota_world_rank=0, bool dakota_mpirun_flag=false)**
  Standard constructor, taking user-specified program options and optionally taking the rank of this process in Dakota’s MPI Comm.
- **~OutputManager ()**
  Destructor that closes streams and other outputs.
- **void close_streams ()**
  helper to close streams during destructor or abnormal abort
- **Graphics & graphics ()**
  retrieve the graphics handler object
- **void parse (const ProgramOptions &prog_opts, const ProblemDescDB &problem_db)**
  Extract environment options from ProblemDescDB and update from late updates to ProgramOptions.
- **void startup_message (const String &start_msg)**
  Set the Dakota startup message ("Running on...")
- **void push_output_tag (const String &iterator_tag, const ProgramOptions &prog_opts, bool force_cout_redirect, bool force_rst_redirect)**
  Update the tag to use on files and rebind any streams as needed.
- **String build_output_tag () const**
  return the full output tag
- **void pop_output_tag ()**
  (Potentially) remove an output context and rebind streams
- **void output_version (std::ostream &os=Cout) const**
  Output the current Dakota version.
- **void output_startup_message (std::ostream &os=Cout) const**
  Output the startup header and time.
- **void output_helper (const String &message, std::ostream &os) const**
  Output only on Dakota world rank 0 (for version, help, etc.)
- **void append_restart (const ParamResponsePair &prp)**
  append a parameter/response set to the restart file
- **void add_datapoint (const Variables &vars, const String &iface, const Response &response)**
  adds data to each window in the 2d graphics and adds a row to the tabular data file based on the results of a model evaluation
- **void create_tabular_datastream (const Variables &vars, const Response &resp)**
  initialize the tabular datastream on iterator leaders
- **void close_tabular ()**
  close tabular datastream
- **void graphics_counter (int cntr)**
  set graphicsCntr equal to cntr
- **int graphics_counter () const**
  return graphicsCntr
- **void tabular_counter_label (const std::string &label)**
  set tabularCntrLabel equal to label
Public Attributes

- `bool graph2DFlag`
  
  whether user requested 2D graphics plots

- `bool tabularDataFlag`
  
  whether user requested tabular data file

- `bool resultsOutputFlag`
  
  whether user requested results data output

- `String tabularDataFile`
  
  filename for tabulation of graphics data

- `String resultsOutputFile`
  
  filename for results data

Private Member Functions

- `void initial_redirects (const ProgramOptions &prog_opts)`
  
  Perform initial output/error redirects from user requests.

- `void read_write_restart (bool restart_requested, bool read_restart_flag, const String &read_restart_filename, size_t stop_restart_eval, const String &write_restart_filename)`
  
  conditionally import evaluations from restart file, then always create or overwrite restart file

Private Attributes

- `int worldRank`
  
  output manager handles rank 0 only output when needed

- `bool mpirunFlag`
  
  some output is only for MPI runs

- `StringArray fileTags`
  
  set of tags for various input/output files (default none)

- `bool redirCalled`
  
  temporary variable to prevent recursive tagging initially

- `ConsoleRedirector coutRedirector`
  
  set of redirections for Dakota::Cout; stores any tagged filename when there are concurrent Iterators

- `ConsoleRedirector cerrRedirector`
  
  set of redirections for Dakota::Cerr; stores any tagged filename when there are concurrent Iterators and error redirection is requested

- `std::vector< boost::shared_ptr< RestartWriter >> restartDestinations`
  
  Stack of active restart destinations; end is the last (active) redirection. All remain open until popped or destroyed.

- `String startupMessage`
  
  message to print at startup when proceeding to instantiate objects

- `Graphics dakotaGraphics`
  
  graphics and tabular data output handler used by meta-iterators, models, and approximations; encapsulated here so destroyed with the OutputManager

- `unsigned short tabularFormat`
tabular format options; see enum
- int graphicsCntr
  used for x axis values in 2D graphics and for 1st column in tabular data
- std::ofstream tabularDataFStream
  file stream for tabulation of graphics data within compute_response
- std::string tabularCntrLabel
  label for counter used in first line comment w/ the tabular data file
- short outputLevel
  output level (for debugging only; not passed in)

13.134.1 Detailed Description
Class to manage redirection of stdout/stderr, keep track of current redir state, and manage rank 0 output. Also manage tabular data output for post-processing with Matlab, Tecplot, etc. and delegate to Graphics for X Windows Graphics.

13.134.2 Constructor & Destructor Documentation
OutputManager ( const ProgramOptions & prog_opts, int dakota_world_rank = 0, bool dakota_mpirun_flag = false )
Standard constructor, taking user-specified program options and optionally taking the rank of this process in Dakota’s MPI_Comm.
  Only get minimal information off ProgramOptions as may be updated later by broadcast.
  References OutputManager::initial_redirects(), OutputManager::mpirunFlag, and Dakota::start_dakota_heartbeat().

13.134.3 Member Function Documentation
void pop_output_tag ()
(Potentially) remove an output context and rebind streams
  For now this assumes the tag is ,<int>
  References OutputManager::build_output_tag(), OutputManager::cerrRedirector, OutputManager::coutRedirector, OutputManager::fileTags, OutputManager::outputLevel, ConsoleRedirector::pop_back(), OutputManager::restartDestinations, and OutputManager::worldRank.
  Referenced by ParallelLibrary::pop_output_tag().

void add_datapoint ( const Variables & vars, const String & iface, const Response & response )
adds data to each window in the 2d graphics and adds a row to the tabular data file based on the results of a model evaluation
  Adds data to each 2d plot and each tabular data column (one for each active variable and for each response function). graphicsCntr is used for the x axis in the graphics and the first column in the tabular data.
  References Response::active_set_request_vector(), Graphics::add_datapoint(), OutputManager::dakotaGraphics, OutputManager::graphicsCntr, OutputManager::tabularDataFStream, and OutputManager::tabularFormat.
  Referenced by DataFitSurrBasedLocalMinimizer::build(), Model::evaluate(), Model::synchronize(), Model::synchronize_nowait(), and DataFitSurrBasedLocalMinimizer::verify().
void create_tabular_datastream ( const Variables & vars, const Response & response )

initialize the tabular datastream on iterator leaders

Opens the tabular data file stream and prints headings, one for each active continuous and discrete variable and one for each response function, using the variable and response function labels. This tabular data is used for post-processing of DAKOTA results in Matlab, Tecplot, etc.

References OutputManager::build_output_tag(), OutputManager::tabularDataFile, OutputManager::tabularDataStream, and OutputManager::tabularFormat.

Referenced by SurrBasedMinimizer::initialize_graphics(), and Iterator::initialize_graphics().

The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp

### 13.135 OutputWriter Class Reference

**Public Member Functions**

- **OutputWriter** (std::ostream *output_stream)
  
  ostream constructor; used to construct a writer to existing stream, e.g., std::cout

- **OutputWriter** (const String &output_filename)
  
  file redirect constructor; opens an overwriting file stream to given name

- const String & filename () const
  
  the (possibly empty) file name for this stream

- std::ostream * output_stream ()
  
  a pointer to the stream, either cout/cerr or a file

**Protected Attributes**

- String outputFilename
  
  the name of the output file (empty when constructed from pointer)

- std::ofstream outputFS
  
  file output stream for console text; only open if string non-empty

- std::ostream * outputStream
  
  pointer to the stream for this writer

### 13.135.1 Detailed Description

Component to manage a redirected output or error stream

The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp

### 13.136 ParallelConfiguration Class Reference

Container class for a set of `ParallelLevel` list iterators that collectively identify a particular multilevel parallel configuration.
Public Member Functions

- **ParallelConfiguration ()**
  *default constructor*
- **ParallelConfiguration (const ParallelConfiguration &pl)**
  *copy constructor*
- **~ParallelConfiguration ()**
  *destructor*
- **ParallelConfiguration & operator= (const ParallelConfiguration &pl)**
  *assignment operator*
- **const ParallelLevel & w_parallel_level () const**
  *return the ParallelLevel corresponding to miPLIter.front()*
- **const ParallelLevel & mi_parallel_level (size_t index=NPOS) const**
  *return the ParallelLevel corresponding to miPLIter[index]*
- **const ParallelLevel & ie_parallel_level () const**
  *return the ParallelLevel corresponding to iePLIter*
- **const ParallelLevel & ea_parallel_level () const**
  *return the ParallelLevel corresponding to eaPLIter*
- **bool w_parallel_level_defined () const**
  *test for definition of world parallel level*
- **bool mi_parallel_level_defined (size_t index=NPOS) const**
  *test for definition of meta-iterator-iterator parallel level*
- **bool ie_parallel_level_defined () const**
  *test for definition of iterator-evaluation parallel level*
- **bool ea_parallel_level_defined () const**
  *test for definition of evaluation-analysis parallel level*
- **ParLevLIter w_parallel_level_iterator () const**
  *return miPLIter.front()*
- **ParLevLIter mi_parallel_level_iterator (size_t index=NPOS) const**
  *return miPLIter[index]*
- **ParLevLIter ie_parallel_level_iterator () const**
  *return iePLIter*
- **ParLevLIter ea_parallel_level_iterator () const**
  *return eaPLIter*
- **size_t mi_parallel_level_index (ParLevLIter pl_iter) const**
  *return the index within miPLIter corresponding to pl_iter*
- **size_t mi_parallel_level_last_index () const**
  *return the index of the last entry in miPLIter*

Private Member Functions

- **void assign (const ParallelConfiguration &pl)**
  *assign the attributes of the incoming pl to this object*
Private Attributes

- short numParallelLevels
  number of parallel levels
- std::vector< ParLevLIter > miPLIter
  list iterator for world level followed by any concurrent iterator partitions (there may be multiple per parallel configuration instance)
- ParLevLIter iePLIter
  list iterator identifying the iterator-evaluation parallelLevel (there can only be one)
- ParLevLIter eaPLIter
  list iterator identifying the evaluation-analysis parallelLevel (there can only be one)
- ParLevLIter endPLIter
  snapshot of the end of ParallelLibrary::parallelLevels; used for detecting when a component of the parallel configuration has been initialized

Friends

- class ParallelLibrary
  the ParallelLibrary class has special access privileges in order to streamline implementation

13.136.1 Detailed Description

Container class for a set of ParallelLevel list iterators that collectively identify a particular multilevel parallel configuration.

Rather than containing the multilevel parallel configuration directly, ParallelConfiguration instead provides a set of list iterators which point into a combined list of ParallelLevels. This approach allows different configurations to reuse ParallelLevels without copying them. A list of ParallelConfigurations is contained in ParallelLibrary (ParallelLibrary::parallelConfigurations).

13.136.2 Member Function Documentation

**const ParallelLevel & mi_parallel_level ( size_t index = _NPOS ) const [inline]**

return the ParallelLevel corresponding to miPLIter[index]

If a meaningful index is not provided, return the last mi parallel level. This is useful within the Model context, for which we need the lowest level partition after any meta-iterator recursions.

References Dakota::_NPOS, and ParallelConfiguration::miPLIter.

Referenced by ApplicationInterface::set_evaluation_communicators().

**ParLevLIter mi_parallel_level_iterator ( size_t index = _NPOS ) const [inline]**

return miPLIter[index]

If a meaningful index is not provided, return the last mi parallel level. This is useful within the Model context, for which we need the lowest level partition after any meta-iterator recursions.

References Dakota::_NPOS, and ParallelConfiguration::miPLIter.

The documentation for this class was generated from the following file:

- ParallelLibrary.hpp
13.137 ParallelDirectApplicInterface Class Reference

Sample derived interface class for testing parallel simulator plug-ins using assign_rep().

Inheritance diagram for ParallelDirectApplicInterface:

```
+-----------------+                  +-----------------+                  +-----------------+
| Interface       |                  | ApplicationInterface |                  | DirectApplicInterface |
|                 +-----------------+                  +-----------------+                  +-----------------+
| ParallelDirectApplicInterface |                  |                    |                    |                    |
```

Public Member Functions

- **ParallelDirectApplicInterface** (const Dakota::ProblemDescDB &problem_db, const MPI_Comm &analysis_comm)
  
  *constructor*

- ∼ParallelDirectApplicInterface()
  
  *destructor*

Protected Member Functions

- int derived_map_ac (const Dakota::String &ac_name)
  
  *execute an analysis code portion of a direct evaluation invocation*

- void derived_map_asynch (const Dakota::ParamResponsePair &pair)
  
  *no-op hides base error; job batching occurs within wait_local_evaluations()*

- void wait_local_evaluations (Dakota::PRPQueue &prp_queue)
  
  *evaluate the batch of jobs contained in prp_queue*

- void test_local_evaluations (Dakota::PRPQueue &prp_queue)
  
  *invokes wait_local_evaluations() (no special nowait support)*

- void set_communicators_checks (int max_eval_concurrency)
  
  *no-op hides default run-time error checks at DirectApplicInterface level*

Private Member Functions

- int text_book (const Dakota::RealVector &c_vars, const Dakota::ShortArray &asv, Dakota::RealVector &fn_vals, Dakota::RealMatrix &fn_grads, Dakota::RealSymMatrixArray &fn_hessians)

  *demo evaluator function for parallel plug-ins*
Additional Inherited Members

13.137.1 Detailed Description

Sample derived interface class for testing parallel simulator plug-ins using assign_rep().

The plug-in ParallelDirectApplicInterface resides in namespace SIM and uses a copy of textbook() to perform parallel parameter to response mappings. It is used to demonstrate plugging in a parallel direct analysis driver into Dakota in library mode. Test input files can then use an analysis driver of "plugin_textbook".

13.137.2 Member Function Documentation

void test_local_evaluations ( Dakota::PRPQueue & prp_queue ) [inline],[protected]
invokes wait_local_evaluations() (no special nowait support)

For use by ApplicationInterface::serve_evaluations_asynch(), which can provide a batch processing capability within message passing schedulers (called using chain ApplicationInterface::serve_evaluations() from Model::serve() from IteratorScheduler::run_iterator()).

References ParallelDirectApplicInterface::wait_local_evaluations().

The documentation for this class was generated from the following files:
- PluginParallelDirectApplicInterface.hpp
- PluginParallelDirectApplicInterface.cpp

13.138 ParallelLevel Class Reference

Container class for the data associated with a single level of communicator partitioning.

Public Member Functions

- ParallelLevel ()
  default constructor
- ParallelLevel (const ParallelLevel &pl)
  copy constructor
- ~ParallelLevel ()
  destructor
- ParallelLevel & operator= (const ParallelLevel &pl)
  assignment operator
- bool dedicated_master () const
  return dedicatedMasterFlag
- bool server_master () const
  return serverMasterFlag
- bool message_pass () const
  return messagePass
- bool idle_partition () const
  return idlePartition
- int num_servers () const
  return numServers
- int processors_per_server () const
return procsPerServer

• int processor_remainder () const
  
return procRemainder

• const MPI_Comm & server_intra_communicator () const
  
return serverIntraComm

• int server_communicator_rank () const
  
return serverCommRank

• int server_communicator_size () const
  
return serverCommSize

• const MPI_Comm & hub_server_intra_communicator () const
  
return hubServerIntraComm

• int hub_server_communicator_rank () const
  
return hubServerCommRank

• int hub_server_communicator_size () const
  
return hubServerCommSize

• const MPI_Comm & hub_server_inter_communicator () const
  
return hubServerInterComm

• MPI_Comm * hub_server_inter_communicators () const
  
return hubServerInterComms

• int server_id () const
  
return serverId

• void read (MPIUnpackBuffer &s)
  
read a ParallelLevel object from a packed MPI buffer

• void write (MPIPackBuffer &s) const
  
write a ParallelLevel object to a packed MPI buffer

• bool null (const MPI_Comm &comm)
  
test comm for MPI_COMM_NULL

• bool special (const MPI_Comm &comm)
  
test comm for special identity that cannot be deallocated

• void clear ()
  
deallocate the communicators in this ParallelLevel

• void alias (const ParallelLevel &pl)
  
assign the attributes of the incoming pl to this object. For communicators, this is a lightweight copy which assigns the same pointer values as the incoming pl, resulting in the same context.

• void copy (const ParallelLevel &pl)
  
deep copy the attributes of the incoming pl to this object using MPI_Comm_dup to create equivalent communicators with a unique context.

• void copy_config (const ParallelLevel &pl)
  
copy the scalar attributes of the incoming pl to this object, omitting communicators
Private Attributes

- bool ownCommFlag
  signals Comm ownership for deallocation
- bool dedicatedMasterFlag
  signals dedicated master partitioning
- bool commSplitFlag
  signals a communicator split was used
- bool serverMasterFlag
  identifies master server processors
- bool messagePass
  flag for message passing at this level, indicating work assignment among servers
- bool idlePartition
  identifies presence of an idle processor partition at this level
- int numServers
  number of servers
- int procsPerServer
  processors per server
- int procRemainder
  proc remainder after equal distribution
- int serverId
  server identifier
- MPI_Comm serverIntraComm
  intracomm. for each server partition
- int serverCommRank
  rank in serverIntraComm
- int serverCommSize
  size of serverIntraComm
- MPI_Comm hubServerIntraComm
  intracomm for all serverCommRank==0 w/ next higher level serverIntraComm
- int hubServerCommRank
  rank in hubServerIntraComm
- int hubServerCommSize
  size of hubServerIntraComm
- MPI_Comm hubServerInterComm
  intercomm. between a server & the hub (on server partitions only)
- MPI_Comm* hubServerInterComms
  intercomm. array on hub processor
Friends

- class ParallelLibrary
  the ParallelLibrary class has special access privileges in order to streamline implementation

13.138.1 Detailed Description

Container class for the data associated with a single level of communicator partitioning.
A list of these levels is contained in ParallelLibrary (ParallelLibrary::parallelLevels), which defines all of the parallelism levels across one or more multilevel parallelism configurations.

13.138.2 Member Function Documentation

void clear() [inline]
deallocate the communicators in this ParallelLevel

This appears to be more robust outside of the destructor due to interactions among managed deallocation and default deallocation (e.g., explicitly freeing a communicator and then default deallocating its handle).

References ParallelLevel::dedicatedMasterFlag, ParallelLevel::hubServerInterComm, ParallelLevel::hubServerInterComms, ParallelLevel::hubServerIntraComm, ParallelLevel::idlePartition, ParallelLevel::numServers, ParallelLevel::ownCommFlag, ParallelLevel::serverId, ParallelLevel::serverIntraComm, and ParallelLevel::special().

The documentation for this class was generated from the following file:
- ParallelLibrary.hpp

13.139 ParallelLibrary Class Reference

Class for partitioning multiple levels of parallelism and managing message passing within these levels.

Public Member Functions

- ParallelLibrary()
  default constructor (used for dummy_lib)

- ParallelLibrary(const MPIManager &mpi_mgr, ProgramOptions &prog_opts, OutputManager &output_mgr)
  stand-alone and default library mode constructor; don’t require options

- ~ParallelLibrary()
  destructor

- const ParallelLevel & init_iterator_communicators(int iterator_servers, int procs_per_iterator, int min_procs_per_iterator, int max_procs_per_iterator, int max_iterator_concurrency, short default_config, short iterator_scheduling, bool peer_dynamicavail)
  split MPI_COMM_WORLD into iterator communicators

- const ParallelLevel & init_evaluation_communicators(int evaluation_servers, int procs_per_evaluation, int min_procs_per_eval, int max_procs_per_eval, int max_evaluation_concurrency, int asynch_local_evaluation_concurrency, short default_config, short evaluation_scheduling, bool peer_dynamicavail)
  split an iterator communicator into evaluation communicators

- const ParallelLevel & init_analysis_communicators(int analysis_servers, int procs_per_analysis, int min_procs_per_analysis, int max_procs_per_analysis, int max_analysis_concurrency, int asynch_local_analysis_concurrency, short default_config, short analysis_scheduling, bool peer_dynamicavail)
split an evaluation communicator into analysis communicators

- void print_configuration ()
  print the parallel level settings for a particular parallel configuration

- void push_output_tag (const ParallelLevel &pl)
  conditionally append an iterator server id tag to the hierarchical output tag, manage restart, and rebind cout/cerr

- void pop_output_tag (const ParallelLevel &pl)
  pop the last output tag and rebind streams as needed; pl isn’t yet used, but may be in the future when we generalize to arbitrary output context switching

- void write_restart (const ParamResponsePair &prp)
  write a parameter/response set to the restart file

- ProgramOptions & program_options ()
  return programOptions reference

- OutputManager & output_manager ()
  return outputManager reference

- void terminate_modelcenter ()
  terminate ModelCenter if running

- void abort_helper (int code)
  finalize MPI with correct communicator for abort

- bool command_line_check () const
  return checkFlag

- bool command_line_pre_run () const
  return preRunFlag

- bool command_line_run () const
  return runFlag

- bool command_line_post_run () const
  return postRunFlag

- bool command_line_user_modes () const
  return userModesFlag

- const String & command_line_pre_run_input () const
  return preRunInput filename

- const String & command_line_pre_run_output () const
  return preRunOutput filename

- const String & command_line_run_input () const
  return runInput filename

- const String & command_line_run_output () const
  return runOutput filename

- const String & command_line_post_run_input () const
  return postRunInput filename

- const String & command_line_post_run_output () const
  return postRunOutput filename

- void send (MPIPackBuffer &send_buff, int dest, int tag, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)
  blocking buffer send at the current communication level
• void **send** (int &send_int, int dest, int tag, const **ParallelLevel** &parent_pl, const **ParallelLevel** &child_pl)
  blocking integer send at the current communication level
• void **isend** (MPIPackBuffer &send_buff, int dest, int tag, MPI_Request &send_req, const **ParallelLevel** &parent_pl, const **ParallelLevel** &child_pl)
  nonblocking buffer send at the current communication level
• void **isend** (int &send_int, int dest, int tag, MPI_Request &send_req, const **ParallelLevel** &parent_pl, const **ParallelLevel** &child_pl)
  nonblocking integer send at the current communication level
• void **recv** (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Status &status, const **ParallelLevel** &parent_pl, const **ParallelLevel** &child_pl)
  blocking buffer receive at the current communication level
• void **recv** (int &recv_int, int source, int tag, MPI_Status &status, const **ParallelLevel** &parent_pl, const **ParallelLevel** &child_pl)
  blocking integer receive at the current communication level
• void **irecv** (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Request &recv_req, const **ParallelLevel** &parent_pl, const **ParallelLevel** &child_pl)
  nonblocking buffer receive at the current communication level
• void **irecv** (int &recv_int, int source, int tag, MPI_Request &recv_req, const **ParallelLevel** &parent_pl, const **ParallelLevel** &child_pl)
  nonblocking integer receive at the current communication level
• void **send** (MPIPackBuffer &send_buff, int dest, int tag, size_t index=NPOS)
  blocking send at the metaiterator-iterator communication level
• void **isend** (int &send_int, int dest, int tag, MPI_Request &send_req, size_t index=NPOS)
  nonblocking send at the metaiterator-iterator communication level
• void **recv** (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Status &status, size_t index=NPOS)
  blocking receive at the metaiterator-iterator communication level
• void **irecv** (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Request &recv_req, size_t index=NPOS)
  nonblocking receive at the metaiterator-iterator communication level
• void **send** (MPIPackBuffer &send_buff, int dest, int tag, size_t index=NPOS)
  blocking send at the metaiterator-iterator communication level
• void **isend** (MPIPackBuffer &send_buff, int dest, int tag, MPI_Request &send_req, size_t index=NPOS)
  nonblocking send at the metaiterator-iterator communication level
• void **recv** (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Status &status, size_t index=NPOS)
  blocking receive at the metaiterator-iterator communication level
• void **irecv** (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Request &recv_req, size_t index=_NPOS)
  nonblocking receive at the metaiterator-iterator communication level
• void **send** (int &send_int, int dest, int tag)
  blocking send at the iterator-evaluation communication level
• void **isend** (int &send_int, int dest, int tag, MPI_Request &send_req)
  nonblocking send at the iterator-evaluation communication level
• void **recv** (int &recv_int, int source, int tag, MPI_Status &status)
blocking receive at the iterator-evaluation communication level
• void irecv_je (int &recv_int, int source, int tag, MPI_Request &recv_req)
nonblocking receive at the iterator-evaluation communication level
• void send_je (MPIPackBuffer &send_buff, int dest, int tag)
blocking send at the iterator-evaluation communication level
• void isend_je (MPIPackBuffer &send_buff, int dest, int tag, MPI_Request &send_req)
nonblocking send at the iterator-evaluation communication level
• void recv_je (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Status &status)
blocking receive at the iterator-evaluation communication level
• void irecv_je (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Request &recv_req)
nonblocking receive at the evaluation-analysis communication level
• void send_ea (int &send_int, int dest, int tag)
blocking send at the evaluation-analysis communication level
• void isend_ea (int &send_int, int dest, int tag, MPI_Request &send_req)
nonblocking send at the evaluation-analysis communication level
• void recv_ea (int &recv_int, int source, int tag, MPI_Status &status)
blocking receive at the evaluation-analysis communication level
• void irecv_ea (int &recv_int, int source, int tag, MPI_Request &recv_req)
nonblocking receive at the evaluation-analysis communication level
• void bcast (int &data, const ParallelLevel &pl)
broadcast an integer across the serverIntraComm of a ParallelLevel
• void bcast (short &data, const ParallelLevel &pl)
broadcast a short integer across the serverIntraComm of a ParallelLevel
• void bcast (MPIPackBuffer &send_buff, const ParallelLevel &pl)
broadcast a MPIPackBuffer across the serverIntraComm of a ParallelLevel
• void bcast (MPIUnpackBuffer &recv_buff, const ParallelLevel &pl)
broadcast a MPIUnpackBuffer across the serverIntraComm of a ParallelLevel
• void bcast_hs (int &data, const ParallelLevel &pl)
broadcast an integer across the hubServerIntraComm of a ParallelLevel
• void bcast_hs (MPIPackBuffer &send_buff, const ParallelLevel &pl)
broadcast a MPIPackBuffer across the hubServerIntraComm of a ParallelLevel
• void bcast_hs (MPIUnpackBuffer &recv_buff, const ParallelLevel &pl)
broadcast a MPIUnpackBuffer across the hubServerIntraComm of a ParallelLevel
• void bcast_w (int &data)
broadcast an integer across MPI_COMM_WORLD
• void bcast_i (int &data, size_t index=NPOS)
broadcast an integer across an iterator communicator
• void bcast_i (short &data, size_t index=NPOS)
broadcast a short integer across an iterator communicator
• void bcast_e (int &data)
broadcast an integer across an evaluation communicator
• void bcast_a (int &data)
broadcast an integer across an analysis communicator
void bcast mi (int &data, size_t index=_NPOS)
  broadcast an integer across a metaiterator-iterator intra communicator

void bcast w (MPIPackBuffer &send_buff)
  broadcast a packed buffer across MPI_COMM_WORLD

void bcast i (MPIPackBuffer &send_buff, size_t index=_NPOS)
  broadcast a packed buffer across an iterator communicator

void bcast e (MPIPackBuffer &send_buff)
  broadcast a packed buffer across an evaluation communicator

void bcast a (MPIPackBuffer &send_buff)
  broadcast a packed buffer across an analysis communicator

void bcast mi (MPIPackBuffer &send_buff, size_t index=_NPOS)
  broadcast a packed buffer across a metaiterator-iterator intra communicator

void bcast w (MPIUnpackBuffer &recv_buff)
  matching receive for packed buffer broadcast across MPI_COMM_WORLD

void bcast i (MPIUnpackBuffer &recv_buff, size_t index=_NPOS)
  matching receive for packed buffer bcast across an iterator communicator

void bcast e (MPIUnpackBuffer &recv_buff)
  matching receive for packed buffer bcast across an evaluation communicator

void bcast a (MPIUnpackBuffer &recv_buff)
  matching receive for packed buffer bcast across an analysis communicator

void barrier w ()
  enforce MPI_Barrier on MPI_COMM_WORLD

void barrier i (size_t index=_NPOS)
  enforce MPI_Barrier on an iterator communicator

void barrier e ()
  enforce MPI_Barrier on an evaluation communicator

void barrier a ()
  enforce MPI_Barrier on an analysis communicator

void reduce sum ea (double *local_vals, double *sum_vals, int num_vals)
  compute a sum over an eval-analysis intra-communicator using MPI_Reduce

void reduce sum a (double *local_vals, double *sum_vals, int num_vals)
  compute a sum over an analysis communicator using MPI_Reduce

void test (MPI_Request &request, int &test_flag, MPI_Status &status)
  test a nonblocking send/receive request for completion

void wait (MPI_Request &request, MPI_Status &status)
  wait for a nonblocking send/receive request to complete

void waitall (int num_recs, MPI_Request *&recv_reqs)
  wait for all messages from a series of nonblocking receives

void waitsome (int num_sends, MPI_Request *&recv_requests, int &num_recs, int *&index_array, MPI_Status *&status_array)
  wait for at least one message from a series of nonblocking receives but complete all that are available
• void free (MPI_Request &request)
  free an MPI_Request
• int world_size () const
  return MPIManager::worldSize
• int world_rank () const
  return MPIManager::worldRank
• bool mpirun_flag () const
  return MPIManager::mpirunFlag
• bool is_null () const
  return dummyFlag
• Real parallel_time () const
  returns current MPI wall clock time
• void parallel_configuration_iterator (ParConfigLIter pc_iter)
  set the current ParallelConfiguration node
• ParConfigLIter parallel_configuration_iterator () const
  return the current ParallelConfiguration node
• const ParallelConfiguration & parallel_configuration () const
  return the current ParallelConfiguration instance
• size_t num_parallel_configurations () const
  returns the number of entries in parallelConfigurations
• bool parallel_configuration_is_complete ()
  identifies if the current ParallelConfiguration has been fully populated
• void increment_parallel_configuration (ParLevLIter mi_pl_iter)
  add a new node to parallelConfigurations and increment currPCIter; limit miPLIter within new configuration to
  mi_pl_iter level
• void increment_parallel_configuration ()
  add a new node to parallelConfigurations and increment currPCIter; copy all of miPLIter into new configuration
• bool w_parallel_level_defined () const
  test current parallel configuration for definition of world parallel level
• bool mi_parallel_level_defined (size_t index=NPOS) const
  test current parallel configuration for definition of meta-iterator-iterator parallel level
• bool ie_parallel_level_defined () const
  test current parallel configuration for definition of iterator-evaluation parallel level
• bool ea_parallel_level_defined () const
  test current parallel configuration for definition of evaluation-analysis parallel level
• ParLevLIter w_parallel_level_iterator ()
  for this level, access through ParallelConfiguration is not necessary
• size_t parallel_level_index (ParLevLIter pl_iter)
  return the index within parallelLevels corresponding to pl_iter
• std::vector< MPIComm > analysis_intra_communicators ()
  return the set of analysis intra communicators for all parallel configurations (used for setting up direct simulation
  interfaces prior to execution time).
Private Member Functions

- void init_mpi_comm ()
  
  convenience function for initializing DAKOTA's top-level MPI communicators, based on dakotaMPIComm

- void initialize_timers ()
  
  initialize DAKOTA and UTILIB timers

- void output_timers ()
  
  conditionally output timers in destructor

- void init_communicators (const ParallelLevel &parent_pl, int num_servers, int procs_per_server, int min_procs_per_server, int max_procs_per_server, int max_concurrency, int asynch_local_concurrency, short default_config, short scheduling_override, bool peer_dynamic_avail)
  
  split a parent communicator into child server communicators

- void split_communicator_dedicated_master (const ParallelLevel &parent_pl, ParallelLevel &child_pl)
  
  split a parent communicator into a dedicated master processor and num_servers child communicators

- void split_communicator_peer_partition (const ParallelLevel &parent_pl, ParallelLevel &child_pl)
  
  split a parent communicator into num_servers peer child communicators (no dedicated master processor)

- void resolve_inputs (ParallelLevel &child_pl, int avail_procs, int min_procs_per_server, int max_procs_per_server, int max_concurrency, int capacity_multiplier, short default_config, short scheduling_override, bool peer_dynamic_avail, bool print_rank)
  
  resolve user inputs into a sensible partitioning scheme

- void bcast (int &data, const MPIComm &comm)
  
  broadcast an integer across a communicator

- void bcast (short &data, const MPIComm &comm)
  
  broadcast a short integer across a communicator

- void bcast (MPIPackBuffer &send_buff, const MPIComm &comm)
  
  send a packed buffer across a communicator using a broadcast

- void bcast (MPIUnpackBuffer &recv_buff, const MPIComm &comm)
  
  matching receive for a packed buffer broadcast

- void barrier (const MPIComm &comm)
  
  enforce MPI_Barrier on comm

- void reduce_sum (double *local_vals, double *sum_vals, int num_vals, const MPIComm &comm)
  
  compute a sum over comm using MPI_Reduce

- void check_error (const String &err_source, int err_code)
  
  check the MPI return code and abort if error

- void alias_as_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)
  
  convenience function for updating child serverIntraComm from parent serverIntraComm (shallow Comm copy)

- void copy_as_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)
  
  convenience function for updating child serverIntraComm from parent serverIntraComm (deep Comm copy)

- void alias_as_hub_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)
  
  convenience function for updating child hubServerIntraComm from parent serverIntraComm (shallow Comm copy)

- void copy_as_hub_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)
  
  convenience function for updating child hubServerIntraComm from parent serverIntraComm (deep Comm copy)
Private Attributes

- **const MPIManager & mpiManager**
  reference to the MPI manager with Dakota’s MPI options
- **ProgramOptions & programOptions**
  *programOptions is non-const due to updates from broadcast*
- **OutputManager & outputManager**
  *Non-const output handler to help with file redirection.*
- **bool dummyFlag**
  prevents multiple MPI_Finalize calls due to dummy_lib
- **bool outputTimings**
  timing info only beyond help/version/check
- **Real startCPUtime**
  start reference for UTILIB CPU timer
- **Real startWCTime**
  start reference for UTILIB wall clock timer
- **Real startMPItime**
  start reference for MPI wall clock timer
- **long startClock**
  start reference for local clock() timer measuring < parent+child CPU
- **std::list< ParallelLevel > parallelLevels**
  the complete set of parallelism levels for managing multilevel parallelism among one or more configurations
- **std::list< ParallelConfiguration > parallelConfigurations**
  the set of parallel configurations which manage list iterators for indexing into parallelLevels
- **ParConfigLIter currPCIter**
  list iterator identifying the current node in parallelConfigurations

### 13.139.1 Detailed Description

Class for partitioning multiple levels of parallelism and managing message passing within these levels.

The ParallelLibrary class encapsulates all of the details of performing message passing within multiple levels of parallelism. It provides functions for partitioning of levels according to user configuration input and functions for passing messages within and across MPI communicators for each of the parallelism levels. If support for other message-passing libraries beyond MPI becomes needed (PVM, ...), then ParallelLibrary would be promoted to a base class with virtual functions to encapsulate the library-specific syntax.

### 13.139.2 Constructor & Destructor Documentation

**ParallelLibrary ( )**

default constructor (used for dummy_lib)

This constructor is used for creation of the global dummy_lib object, which is used to satisfy initialization requirements when the real ParallelLibrary object is not available.
ParallelLibrary (const MPIManager & mpi_mgr, ProgramOptions & prog_opts, OutputManager & output_mgr)

stand-alone and default library mode constructor; don’t require options
   library mode constructor accepting communicator
TODO: Update comment.
   Same constructor is used for executable and library environments and sequencing of object construction is
   ordered, so no need to separately get updates off command line (programOptions)
   References ParallelLibrary::init_mpi_comm(), and ParallelLibrary::initialize_timers().

13.139.3 Member Function Documentation

void push_output_tag (const ParallelLevel & pl)

conditionally append an iterator server id tag to the hierarchical output tag, manage restart, and rebind cout/cerr
   If the user has specified the use of files for DAKOTA standard output and/or standard error, then bind these
   filenames to the Cout/Cerr macros. In addition, if concurrent iterators are to be used, create and tag multiple output
   streams in order to prevent jumbled output. Manage restart file(s) by processing any incoming evaluations from
   an old restart file and by setting up the binary output stream for new evaluations. Only master iterator processor(s)
   read & write restart information. This function must follow init_iterator_communicators so that restart can be
   managed properly for concurrent iterator strategies. In the case of concurrent iterators, each iterator has its own
   restart file tagged with iterator number.
   References ParallelLibrary::bcast(), ParallelLevel::dedicatedMasterFlag, OutputManager::graph2DFlag, ParallelLevel::hubServerCommRank, ParallelLevel::hubServerCommSize, ParallelLevel::hubServerIntraComm, ParallelLevel::numServers, ParallelLibrary::outputManager, ParallelLibrary::programOptions, OutputManager::push_output_tag(), OutputManager::resultsOutputFile, OutputManager::resultsOutputFlag, ParallelLevel::serverCommRank, ParallelLevel::serverId, MPIPackBuffer::size(), OutputManager::tabularDataFile, and OutputManager::tabularDataFlag.
   Referenced by Environment::construct(), and IteratorScheduler::partition().

void terminate_modelcenter ()

terminate ModelCenter if running
   Close streams associated with manage_outputs and manage_restart and terminate any additional services that
   may be active.
   References Dakota::abort_handler(), Dakota::dc_ptr_int, and Dakota::mc_ptr_int.
   Referenced by ParallelLibrary::~ParallelLibrary().

void increment_parallel_configuration (ParLevIter mi_pl_iter) [inline]

add a new node to parallelConfigurations and increment currPCIter; limit miPLIters within new configuration to
   mi_pl_iter level
   Called from the ParallelLibrary ctor and from Model::init_communicators(). An increment is performed for each
   Model initialization except the first (which inherits the world level from the first partial configuration).
   References ParallelLibrary::currPCIter, ParallelConfiguration::eaPLIter, ParallelConfiguration::endPLIter, ParallelConfiguration::iePLIter, ParallelConfiguration::miPLIter, ParallelConfiguration::numParallelLevels, ParallelLibrary::parallelConfigurations, and ParallelLibrary::parallelLevels.
   Referenced by Iterator::init_communicators(), and Model::init_communicators().
void init_mpi_comm() [private]

convenience function for initializing DAKOTA's top-level MPI communicators, based on dakotaMPIComm

shared function for initializing based on passed MPI_Comm

References Dakota::abort_handler(), MPIManager::dakota_mpi_comm(), ParallelLibrary::increment_parallel_configuration(), ParallelLibrary::mpiManager, MPIManager::mpirun_flag(), ParallelLevel::numServers, ParallelLibrary::outputManager, ParallelLibrary::parallelLevels, ParallelLevel::procsPerServer, ParallelLevel::serverCommRank, ParallelLevel::serverCommSize, ParallelLevel::serverId, ParallelLevel::serverIntraComm, ParallelLevel::serverMasterFlag, ParallelLibrary::startMPItime, OutputManager::startup_message(), MPIManager::world_rank(), and MPIManager::world_size.

Referenced by ParallelLibrary::ParallelLibrary().

void init_communicators ( const ParallelLevel & parent_pl, int num_servers, int procs_per_server, int min_procs_per_server, int max_procs_per_server, int max_concurrency, int asynch_local_concurrency, short default_config, short scheduling_override, bool peer_dynamic_avail ) [private]

split a parent communicator into child server communicators

Split parent communicator into concurrent child server partitions as specified by the passed parameters. This constructs new child intra-communicators and parent-child inter-communicators. This fn is called from Meta-Iterators and NestedModel for the concurrent iterator level and from ApplicationInterface::init_communicators() for the concurrent evaluation and concurrent analysis levels.

References ParallelLibrary::currPCIter, ParallelLevel::dedicatedMasterFlag, ParallelLevel::messagePass, ParallelLevel::numServers, ParallelLibrary::parallelLevels, ParallelLevel::procsPerServer, ParallelLibrary::resolve_inputs(), ParallelLevel::serverCommRank, ParallelLevel::serverCommSize, ParallelLibrary::split_communicator_dedicated_master(), and ParallelLibrary::split_communicator_peer_partition().

Referenced by ParallelLibrary::init_analysis_communicators(), ParallelLibrary::init_evaluation_communicators(), and ParallelLibrary::init_iterator_communicators().

void resolve_inputs ( ParallelLevel & child_pl, int avail_procs, int min_procs_per_server, int max_procs_per_server, int max_concurrency, int capacity_multiplier, short default_config, short scheduling_override, bool peer_dynamic_avail, bool print_rank ) [private]

resolve user inputs into a sensible partitioning scheme

This function is responsible for the “auto-configure” intelligence of DAKOTA. It resolves a variety of inputs and overrides into a sensible partitioning configuration for a particular parallelism level. It also handles the general case in which a user’s specification request does not divide out evenly with the number of available processors for the level. If num_servers & procs_per_server are both nondefault, then the former takes precedence.

References Dakota::abort_handler(), ParallelLevel::dedicatedMasterFlag, ParallelLevel::numServers, ParallelLevel::procRemainder, and ParallelLevel::procPerServer.

Referenced by ParallelLibrary::init_communicators().

The documentation for this class was generated from the following files:
- ParallelLibrary.hpp
- ParallelLibrary.cpp

13.140 ParamResponsePair Class Reference

Container class for a variables object, a response object, and an evaluation id.
Public Member Functions

- **ParamResponsePair ()**
  
  default constructor

- **ParamResponsePair (const Variables &vars, const String &interface_id, const Response &response, bool deep_copy=false)**
  
  alternate constructor for temporaries

- **ParamResponsePair (const Variables &vars, const String &interface_id, const Response &response, const int eval_id, bool deep_copy=true)**
  
  standard constructor for history uses

- **ParamResponsePair (const ParamResponsePair &pair)**
  
  copy constructor

- **∼ParamResponsePair ()**
  
  destructor

- **ParamResponsePair & operator= (const ParamResponsePair &pair)**
  
  assignment operator

- **void read (std::istream &s)**
  
  read a ParamResponsePair object from an std::istream

- **void write (std::ostream &s) const**
  
  write a ParamResponsePair object to an std::ostream

- **void read.annotated (std::istream &s)**
  
  read a ParamResponsePair object in annotated format from an std::istream

- **void write.annotated (std::ostream &s) const**
  
  write a ParamResponsePair object in annotated format to an std::ostream

- **void write.tabular (std::ostream &s, unsigned short tabular_format) const**
  
  write a ParamResponsePair object in tabular format (all variables active/inactive) to an std::ostream

- **void write.tabular.labels (std::ostream &s, unsigned short tabular_format) const**
  
  write PRP labels in tabular format to an std::ostream

- **void read (MPIUnpackBuffer &s)**
  
  read a ParamResponsePair object from a packed MPI buffer

- **void write (MPIPackBuffer &s) const**
  
  write a ParamResponsePair object to a packed MPI buffer

- **int eval_id () const**
  
  return the evaluation identifier

- **void eval_id (int id)**
  
  set the evaluation identifier

- **const String & interface_id () const**
  
  return the interface identifier from evalInterfaceIds

- **void interface_id (const String &id)**
  
  set the interface identifier within evalInterfaceIds

- **const IntStringPair & eval_interface_ids () const**
  
  return the aggregate eval/interface identifier from the response object

- **const Variables & variables () const**
  
  return the parameters object
• void variables (const Variables &vars)
  set the parameters object
• const Response & response () const
  return the response object
• void response (const Response &resp)
  set the response object
• const ActiveSet & active_set () const
  return the active set object from the response object
• void active_set (const ActiveSet &set)
  set the active set object within the response object

Private Member Functions
• template<class Archive >
  void serialize (Archive &ar, const unsigned int version)
  serialize the PRP: write and read are symmetric for this class

Private Attributes
• Variables prpVariables
  the set of parameters for the function evaluation
• Response prpResponse
  the response set for the function evaluation
• IntStringPair evalInterfaceIds
  the evalInterfaceIds aggregate

Friends
• class boost::serialization::access
  allow boost access to serialize this class
• bool operator== (const ParamResponsePair &pair1, const ParamResponsePair &pair2)
  equality operator
• bool operator!= (const ParamResponsePair &pair1, const ParamResponsePair &pair2)
  inequality operator

13.140.1 Detailed Description
Container class for a variables object, a response object, and an evaluation id.

ParamResponsePair provides a container class for association of the input for a particular function evaluation (a variables object) with the output from this function evaluation (a response object), along with an evaluation identifier. This container defines the basic unit used in the data pairs cache, in restart file operations, and in a variety of scheduling algorithm queues. With the advent of STL, replacement of arrays of this class with map<> and pair<> template constructs may be possible (using map<pair<int,String>, pair<Variables,Response> >, for example), assuming that deep copies, I/O, alternate constructors, etc., can be adequately addressed. Boost tuple<> may also be a candidate.
13.140. **Constructor & Destructor Documentation**

**ParamResponsePair** ( const Variables & *vars*, const String & *interface_id*, const Response & *response*,
bool *deep_copy = false*) [inline]

alternate constructor for temporaries

Uses of this constructor often employ the standard Variables and Response copy constructors to share representations since this constructor is commonly used for search pairs (which are local instantiations that go out of scope prior to any changes to values; i.e., they are not used for history).

**ParamResponsePair** ( const Variables & *vars*, const String & *interface_id*, const Response & *response*,
const int *eval_id*, bool *deep_copy = true*) [inline]

standard constructor for history uses

Uses of this constructor often do not share representations since deep copies are used when history mechanisms (e.g., data_pairs and beforeSynchCorePRPQueue) are involved.

13.140.3 **Member Function Documentation**

**void read** ( MPIUnpackBuffer & *s*) [inline]

read a ParamResponsePair object from a packed MPI buffer

interfaceId is omitted since master processor retains interface ids and communicates asv and response data only with slaves.

References ParamResponsePair::evalInterfaceIds, ParamResponsePair::prpResponse, and ParamResponsePair::prpVariables.

**void write** ( MPIPackBuffer & *s*) const [inline]

write a ParamResponsePair object to a packed MPI buffer

interfaceId is omitted since master processor retains interface ids and communicates asv and response data only with slaves.

References ParamResponsePair::evalInterfaceIds, ParamResponsePair::prpResponse, and ParamResponsePair::prpVariables.

13.140.4 **Member Data Documentation**

**IntStringPair evalInterfaceIds** [private]

the evalInterfaceIds aggregate

the function evaluation identifier (assigned from Interface::evalIdCntr) is paired with the interface used to generate the response object. Used in PRPCache id_vars_set_compare to prevent duplicate detection on results from different interfaces. evalInterfaceIds belongs here rather than in Response since some Response objects involve consolidation of several fn evals (e.g., Model::synchronize_derivatives()) that are not, in total, generated by a single interface. The prPair, on the other hand, is used for storage of all low level fn evals that get evaluated in ApplicationInterface::map().

Referenced by ParamResponsePair::eval_id(), ParamResponsePair::eval_interface_ids(), ParamResponsePair::interface_id(), ParamResponsePair::operator==(), Dakota::operator==(), ParamResponsePair::read(), and ParamResponsePair::write().

The documentation for this class was generated from the following file:

- ParamResponsePair.hpp
13.141 ParamStudy Class Reference

Class for vector, list, centered, and multidimensional parameter studies.

Inheritance diagram for ParamStudy:

```
  ParamStudy
    |  PStudyDACE
    |  Analyzer
    |  Iterator
```

Public Member Functions

- **ParamStudy** (ProblemDescDB &problem_db, Model &model)
  
  constructor

- **~ParamStudy** ()
  
  destructor

- **bool resize ()**

  reinitializes iterator based on new variable size

- **void pre_run ()**

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

- **void core_run ()**

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

- **void post_input ()**

  read tabular data for post-run mode

- **void post_run (std::ostream &s)**

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Private Member Functions

- **void sample ()**

  performs the parameter study by sampling from a list of points

- **void vector_loop ()**

  performs the parameter study by sampling along a vector, starting from an initial point followed by numSteps increments along continuous/discrete step vectors

- **void centered_loop ()**

  performs a number of plus and minus offsets for each parameter centered about an initial point

- **void multidim_loop ()**

  performs a full factorial combination for all intersections defined by a set of multidimensional partitions
• bool load_distribute_points (const String &points_filename, unsigned short tabular_format, bool active_only)
  load list of points from data file and distribute among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints
• template<typename OrdinalType , typename ScalarTypeA , typename ScalarTypeC , typename ScalarTypeDI , typename ScalarTypeDS , typename ScalarTypeDR >
  bool distribute (const Teuchos::SerialDenseVector< OrdinalType, ScalarTypeA > &all_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeC > &c_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeDI > &di_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeDS > &ds_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeDR > &dr_data)
  distributes incoming all vector in standard variable ordering among continuous, discrete int, discrete string, and discrete real vectors
• template<typename ScalarType >
  bool distribute (const std::vector< ScalarType > &all_data, std::vector< ScalarType > &c_data, std::vector< ScalarType > &di_data, std::vector< ScalarType > &ds_data, std::vector< ScalarType > &dr_data)
  distributes incoming all array in standard variable ordering among continuous, discrete int, discrete string, and discrete real arrays
• bool distribute_list_of_points (const RealVector &list_of_pts)
  distributes list of pts coming from user spec among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints
• void final_point_to_step_vector ()
  compute step vectors from finalPoint, initial points, and numSteps
• void distribute_partitions ()
  compute step vectors from {cont,discInt,discString,discReal}VarPartitions and global bounds
• bool check_num_steps (int num_steps)
  perform error checks on numSteps
• bool check_step_vector (const RealVector &step_vector)
  perform error checks on step
• bool check_final_point (const RealVector &final_pt)
  perform error checks on finalPoint
• bool check_steps_per_variable (const IntVector &steps_per_var)
  perform error checks on stepsPerVariable
• bool check_variable_partitions (const UShortArray &partitions)
  perform error checks on variable partitions
• bool check_finite_bounds ()
  check for finite variable bounds within iteratedModel, as required for computing partitions of finite ranges
• bool check_ranges_sets (int num_steps)
  sanity check for vector parameter study
• bool check_ranges_sets (const IntVector &c_steps, const IntVector &di_steps, const IntVector &ds_steps, const IntVector &dr_steps)
  sanity check for centered parameter study
• bool check_sets (const IntVector &c_steps, const IntVector &di_steps, const IntVector &ds_steps, const IntVector &dr_steps)
  sanity check for increments along int/real set dimensions
• int integer_step (int range, int num_steps) const
  check for integer remainder and return step
• int index_step (size_t start, size_t end, int num_steps) const
check for out of bounds and index remainder and return step

- void c_step (size_t c_index, int increment, Variables &vars)
  helper function for performing a continuous step in one variable
- void dri_step (size_t di_index, int increment, Variables &vars)
  helper function for performing a discrete step in an integer range variable
- void dsi_step (size_t di_index, int increment, const IntSet &values, Variables &vars)
  helper function for performing a discrete step in an integer set variable
- void dss_step (size_t ds_index, int increment, const StringSet &values, Variables &vars)
  helper function for performing a discrete step in a string set variable
- void dsr_step (size_t dr_index, int increment, const RealSet &values, Variables &vars)
  helper function for performing a discrete step in a real set variable
- void reset (Variables &vars)
  reset vars to initial point (center)
- void centered_header (const String &type, size_t var_index, int step, size_t hdr_index)
  store a centered parameter study header within allHeaders

Private Attributes

- size_t numEvals
  total number of parameter study evaluations computed from specification
- RealVectorArray listCVPoints
  array of continuous evaluation points for the list parameter study
- IntVectorArray listDIVPoints
  array of discrete int evaluation points for the list parameter study
- StringMulti2DArray listDSVPoints
  array of discrete string evaluation points for the list parameter study
- RealVectorArray listDRVPoints
  array of discrete real evaluation points for the list parameter study
- RealVector initialCVPoint
  the continuous start point for vector and centered parameter studies
- IntVector initialDIVPoint
  the discrete int start point for vector and centered parameter studies
- StringMultiArray initialDSVPoint
  the discrete string start point for vector and centered parameter studies
- RealVector initialDRVPoint
  the discrete real start point for vector and centered parameter studies
- RealVector finalCVPoint
  the continuous ending point for vector parameter study
- IntVector finalDIVPoint
  the discrete int range value or set index ending point for vector parameter study
- IntVector finalDSVPoint
  the discrete string set index ending point for vector parameter study
- IntVector finalDRVPoint
the discrete real set index ending point for vector_parameter_study

- RealVector contStepVector
  the n-dimensional continuous increment

- IntVector discIntStepVector
  the n-dimensional discrete integer range value or set index increment

- IntVector discStringStepVector
  the n-dimensional discrete string set index increment

- IntVector discRealStepVector
  the n-dimensional discrete real set index increment

- int numSteps
  the number of times continuous/discrete step vectors are applied for vector_parameter_study (a specification option)

- IntVector contStepsPerVariable
  number of offsets in the plus and the minus direction for each continuous variable in a centered_parameter_study

- IntVector discIntStepsPerVariable
  number of offsets in the plus and the minus direction for each discrete integer variable in a centered_parameter_study

- IntVector discStringStepsPerVariable
  number of offsets in the plus and the minus direction for each discrete string variable in a centered_parameter_study

- IntVector discRealStepsPerVariable
  number of offsets in the plus and the minus direction for each discrete real variable in a centered_parameter_study

- UShortArray contVarPartitions
  number of partitions for each continuous variable in a multidim_parameter_study

- UShortArray discIntVarPartitions
  number of partitions for each discrete integer variable in a multidim_parameter_study

- UShortArray discStringVarPartitions
  number of partitions for each discrete string variable in a multidim_parameter_study

- UShortArray discRealVarPartitions
  number of partitions for each discrete real variable in a multidim_parameter_study

Additional Inherited Members

13.141.1 Detailed Description

Class for vector, list, centered, and multidimensional parameter studies.

The ParamStudy class contains several algorithms for performing parameter studies of different types. The vector parameter study steps along an n-dimensional vector from an arbitrary initial point to an arbitrary final point in a specified number of steps. The centered parameter study performs a number of plus and minus offsets in each coordinate direction around a center point. A multidimensional parameter study fills an n-dimensional hypercube based on bounds and a specified number of partitions for each dimension. And the list parameter study provides for a user specification of a list of points to evaluate, which allows general parameter investigations not fitting the structure of vector, centered, or multidim parameter studies.
13.141.2 Member Function Documentation

void pre_run( ) [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s pre_run(), if implemented, typically before performing its own implementation steps.

Reimplemented from Analyzer.

References Dakota::abort_handler(), SharedVariablesData::active_components_totals(), Analyzer::allHeaders, Analyzer::allVariables, ParamStudy::centered_loop(), Variables::continuous_variables(), ParamStudy::contStepsPerVariable, ParamStudy::contStepVector, ParamStudy::contVarPartitions, Dakota::copy_data(), Model::current_variables(), ParamStudy::discIntStepsPerVariable, ParamStudy::discIntStepVector, ParamStudy::discIntVarPartitions, ParamStudy::discRealStepsPerVariable, ParamStudy::discRealStepVector, ParamStudy::discRealVarPartitions, Variables::discrete_int_variables(), Variables::discrete_real_variables(), Variables::discrete_string_variables(), ParamStudy::discStringStepsPerVariable, ParamStudy::discStringStepVector, ParamStudy::discStringVarPartitions, ParamStudy::distribute_partitions(), ParamStudy::final_point_to_step_vector(), ParamStudy::finalCVPoint, ParamStudy::finalDIVPoint, ParamStudy::finalDREVPoint, ParamStudy::finalDSVPoint, ParamStudy::initialCVPoint, ParamStudy::initialDIVPoint, ParamStudy::initialDSVPoint, ParamStudy::initialDRVPoint, Iterator::iteratedModel, Iterator::method_enum_to_string(), Iterator::methodName, ParamStudy::multidim_loop(), Analyzer::numDiscreteStringVars, ParamStudy::numEvals, ParamStudy::numSteps, Iterator::outputLevel, Analyzer::pre_run(), ParamStudy::sample(), Variables::shared_data(), Dakota::svd(), ParamStudy::vector_loop(), and Dakota::write_ordered().

void core_run( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, Iterator::methodName, Analyzer::numLSqTerms, Analyzer::numObjFns, and Iterator::subIteratorFlag.

void post_run ( std::ostream & s ) [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s post_run(), typically after performing its own implementation steps.

Reimplemented from Analyzer.

References Analyzer::allResponses, Analyzer::allVariables, SensAnalysisGlobal::compute_correlations(), Model::discrete_set_string_values(), Iterator::iteratedModel, Iterator::methodName, Analyzer::post_run(), PStudyDACE::pStudyDACESensGlobal, and Iterator::subIteratorFlag.

bool load_distribute_points ( const String & points_filename, unsigned short tabular_format, bool active_only ) [private]

load list of points from data file and distribute among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints
Load from file and distribute points; using this function to manage construction of the temporary arrays. Historically all data was read as a real (mixture of values and indices), but now points file is valued-based (reals, integers, strings) so file input matches tabular data output. Return false on success.

References Dakota::NPOS, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Variables::copy(), Model::current_variables(), Model::discrete_int_lower_bounds(), Model::discrete_int_upper_bounds(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Iterator::iteratedModel, ParamStudy::listCVPoints, ParamStudy::listDIVPoints, ParamStudy::listDRVPoints, ParamStudy::listDSVPoints, Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, ParamStudy::numEvals, and Dakota::set_value_to_index().

Referenced by ParamStudy::ParamStudy().

bool distribute_list_of_points ( const RealVector & list_of_pts ) [private]
distributes list_of_pts coming from user spec among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints

Parse list of points into typed data containers; list_of_pts will contain values for continuous and discrete integer range, but indices for all discrete set types (int, string, real)

References Model::discrete_int_sets(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), ParamStudy::distribute(), Iterator::iteratedModel, ParamStudy::listCVPoints, ParamStudy::listDIVPoints, ParamStudy::listDSVPoints, ParamStudy::listDRVPoints, Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, ParamStudy::numEvals, and Dakota::set_index_to_value().

Referenced by ParamStudy::ParamStudy().

The documentation for this class was generated from the following files:

- ParamStudy.hpp
- ParamStudy.cpp

13.142 partial_prp_equality Struct Reference

predicate for comparing ONLY the interfaceId and Vars attributes of PRPair

Public Member Functions

- bool operator() (const ParamResponsePair &database_pr, const ParamResponsePair &search_pr) const

13.142.1 Detailed Description

predicate for comparing ONLY the interfaceId and Vars attributes of PRPair

The documentation for this struct was generated from the following file:

- PRPMultiIndex.hpp

13.143 partial_prp_hash Struct Reference

wrapper to delegate to the ParamResponsePair hash_value function
Public Member Functions

- std::size_t operator() (const ParamResponsePair &prp) const
  access operator

13.143.1 Detailed Description

Wrapper to delegate to the ParamResponsePair hash_value function

The documentation for this struct was generated from the following file:

- PRPMultiIndex.hpp

13.144 PebbldBranching Class Reference

Main Branching class for the PEBBL-based Minimizer.
Inherits branching.

Public Member Functions

- PebbldBranching ()
  Default Constructor.
- ~PebbldBranching ()
  Destructor.
- pebbl::branchSub * blankSub ()
  Method that returns an empty Sub-Branch.
- void setModel (Model &model)
- void setIterator (Iterator &iterator)

Protected Attributes

- Model parentModel
  Original model, before branching.
- Iterator nlpSolver
  Solver to be used at root node.
- RealVector cont_vars
  Initial variable values for root node.
- RealVector lower_bounds
  Lower bounds for root node.
- RealVector upper_bounds
  Upper bounds for root node.

Friends

- class PebbldBranchSub
13.145. **PEBBLDBRANCHSUB CLASS REFERENCE**

### 13.144.1 Detailed Description

Main Branching class for the PEBBL-based Minimizer.

The documentation for this class was generated from the following files:

- PEBBLBranching.hpp
- PEBBLBranching.cpp

### 13.145 PebbldBranchSub Class Reference

Sub Branch class for the PEBBL-based Minimizer.

Inherits branchSub.

**Public Member Functions**

- **PebbldBranchSub ()**
  Constructor.
- **~PebbldBranchSub ()**
  Destructor.
- **PebbldBranching * global () const**
  Returns a reference to the corresponding main Branching object.
- **pebbl::branching * bGlobal () const**
  Returns a reference to the corresponding main Branching object.
- **void setGlobalInfo (PebbldBranching *global_)**
  Method that sets up the main Branching object.
- **void setRootComputation ()**
  Method that is called when declaring the current node as a root node.
- **void boundComputation (double *controlParam)**
  Method that does the Bounding Operation. In other words, it calls the optimization algorithm on the relaxed domain.
- **bool candidateSolution ()**
  Method called after the bounding operation, returns true if the bounding resulted in a possible solution to the original non-relaxed problem.
- **pebbl::solution * extractSolution ()**
  Method that returns a PEBBL-based solution.
- **int splitComputation ()**
  Method that determines how many branches are created and how. Returns the number of branches created from this object.
- **pebbl::branchSub * makeChild (int whichChild)**
  Method that returns a new PebbldBranchSub object based on Objective Function improvements and the number of branches.
- **void pebbldSubAsChildOf (PebbldBranchSub *parent, int splitVar, int whichChild, std::vector<double> _candidate_x, RealVector _lower_bounds, RealVector _upper_bounds)**
  Method that creates a new PebbldBranching object.
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Protected Attributes

- **PebbldBranching** ∗ globalPtr
  
  *Pointer referring to all info passed to subproblem.*

- **Model** subModel
  
  *Model used for sub-problem.*

- **Iterator** subNLP Solver
  
  *Solver used for sub-problems.*

- **std::vector<double>** candidate
  
  *Candidate solution after solving sub-problem (also the bound)*

- **double** candidate_objFn
  
  *Objective value at the candidate solution.*

- **int** splitVar
  
  *Variable to branch on.*

- **RealVector** cont vars
  
  *Initial variable values for sub-problem.*

- **RealVector** lower bounds
  
  *Lower bounds for sub-problem.*

- **RealVector** upper bounds
  
  *Upper bounds for sub-problem.*

Friends

- class **PebbldBranching**

13.145.1 Detailed Description

Sub Branch class for the PEBBL-based Minimizer.

The documentation for this class was generated from the following files:

- PEBBLBranching.hpp
- PEBBLBranching.cpp

13.146 PebbldMinimizer Class Reference

Wrapper class for experimental PebbldMinimizer.

Inheritance diagram for PebbldMinimizer:

```
  Iterator
     |        
     v        
Minimizer
    |        
    v        
PebbldMinimizer
```
Public Member Functions

- PebblMinimizer (ProblemDescDB &problem_db, Model &model)
  *standard constructor*
- PebblMinimizer (Model &model)
  *Constructor.*
- PebblMinimizer (Model &model, int random_seed, int max_iter, int max_eval)
  *Constructor.*
- ~PebblMinimizer ()
  *Destructor.*

Protected Member Functions

- void core_run ()
  *Calls the Pebbl Branch and Bound solver.*
- void print_results (std::ostream &s)
  *Redefinition of default results printing.*

Private Attributes

- PebblBranching * branchAndBound
  *Object that implements the branching and bounding logic.*
- Iterator subProbMinimizer
  *Minimizer used to solve the subproblem on each branch.*

Additional Inherited Members

13.146.1 Detailed Description

Wrapper class for experimental PebblMinimizer.

13.146.2 Constructor & Destructor Documentation

PebblMinimizer ( Model & model )

Constructor.

Parameters

| model  | DAKOTA Model object |

PebblMinimizer ( Model & model, int random_seed, int max_iter, int max_eval )

Constructor.

PebblMinimizer Constructor
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#### Parameters

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<td>random_seed</td>
<td>Random Seed</td>
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<td>Maximum number of iterations</td>
</tr>
<tr>
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</tr>
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#### 13.146.3 Member Function Documentation

**void core_run ( ) [protected], [virtual]**

Calls the Pebbl Branch and Bound solver. redefines default iterator logic to execute branch and bound and extract optimization results. Reimplemented from Iterator. References Iterator::bestResponseArray, Iterator::bestVariablesArray, PebbldMinimizer::branchAndBound, and Minimizer::numContinuousVars.

**void print_results ( std::ostream & s ) [protected], [virtual]**

Redefinition of default results printing. Redefines default iterator results printing to include optimization results (objective functions and constraints). Reimplemented from Iterator. References Dakota::abort_handler(), Iterator::activeSet, Minimizer::archive_allocate_best(), Minimizer::archive_best(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Dakota::data_pairs, Model::interface_id(), Iterator::iteratedModel, Dakota::lookup_by_val(), Minimizer::numFunctions, Minimizer::numUserPrimaryFns, Minimizer::optimizationFlag, and ActiveSet::request_values().

The documentation for this class was generated from the following files:

- PEBBLMinimizer.hpp
- PEBBLMinimizer.cpp

#### 13.147 PecosApproximation Class Reference

Derived approximation class for global basis polynomials. Inheritance diagram for PecosApproximation:

```
Approximation
  PecosApproximation
```

**Public Member Functions**

- **PecosApproximation ()**
  default constructor
- **PecosApproximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)**
  standard ProblemDescDB-driven constructor
• **PecosApproximation** (const `SharedApproxData` &shared_data)
  alternate constructor

• **~PecosApproximation** ()
  destructor

• **void expansion_coefficient_flag** (bool coeff_flag)
  set `pecosBasisApprox.configOptions.expansionCoeffFlag`

• **bool expansion_coefficient_flag** () const
  get `pecosBasisApprox.configOptions.expansionCoeffFlag`

• **void expansion_gradient_flag** (bool grad_flag)
  set `pecosBasisApprox.configOptions.expansionGradFlag`

• **bool expansion_gradient_flag** () const
  get `pecosBasisApprox.configOptions.expansionGradFlag`

• **void compute_component_effects** ()
  Performs global sensitivity analysis using Sobol’ Indices by computing component (main and interaction) effects.

• **void compute_total_effects** ()
  Performs global sensitivity analysis using Sobol’ Indices by computing total effects.

• **const Pecos::RealVector & sobol_indices** () const
  return polyApproxRep->sobolIndices

• **const Pecos::RealVector & total_sobol_indices** () const
  return polyApproxRep->totalSobolIndices

• **Pecos::ULongULongMap sparse_sobol_index_map** () const
  return RegressOrthogPolyApproximation::sparseSobolIndexMap

• **const Pecos::RealVector & dimension_decay_rates** () const
  return OrthogPolyApproximation::decayRates

• **void allocate_arrays** ()
  invoke Pecos::PolynomialApproximation::allocate_arrays()

• **Real mean** ()
  return the mean of the expansion, treating all variables as random

• **Real mean** (const Pecos::RealVector &x)
  return the mean of the expansion for a given parameter vector, treating a subset of the variables as random

• **const Pecos::RealVector & mean_gradient** ()
  return the gradient of the expansion mean for a given parameter vector, treating all variables as random

• **const Pecos::RealVector & mean_gradient** (const Pecos::RealVector &x, const Pecos::SizetArray &dvv)
  return the gradient of the expansion mean for a given parameter vector and given DVV, treating a subset of the variables as random

• **Real variance** ()
  return the variance of the expansion, treating all variables as random

• **Real variance** (const Pecos::RealVector &x)
  return the variance of the expansion for a given parameter vector, treating a subset of the variables as random

• **const Pecos::RealVector & variance_gradient** ()
  return the gradient of the expansion variance for a given parameter vector, treating all variables as random

• **const Pecos::RealVector & variance_gradient** (const Pecos::RealVector &x, const Pecos::SizetArray &dvv)
return the gradient of the expansion variance for a given parameter vector and given DVV, treating a subset of the variables as random

- Real \texttt{covariance (PecosApproximation \&pecos\_approx\_2)}
  return the covariance between two response expansions, treating all variables as random

- Real \texttt{covariance (const Pecos::RealVector \&x, PecosApproximation \&pecos\_approx\_2)}
  return the covariance between two response expansions, treating a subset of the variables as random

- Real \texttt{delta\_covariance (PecosApproximation \&pecos\_approx\_2)}
  return the change in covariance between two response expansions, treating all variables as random

- Real \texttt{delta\_covariance (const Pecos::RealVector \&x, PecosApproximation \&pecos\_approx\_2)}
  return the change in covariance between two response expansions, treating a subset of the variables as random

- Real \texttt{delta\_mean ()}
  return the change in mean between two response expansions, treating all variables as random

- Real \texttt{delta\_mean (const RealVector \&x)}
  return the change in mean between two response expansions, treating a subset of variables as random

- Real \texttt{delta\_std\_deviation ()}
  return the change in standard deviation between two response expansions, treating all variables as random

- Real \texttt{delta\_std\_deviation (const RealVector \&x)}
  return the change in standard deviation between two response expansions, treating a subset of variables as random

- Real \texttt{delta\_beta (bool cdf\_flag, Real z\_bar)}
  return the change in reliability index (mapped from z\_bar) between two response expansions, treating all variables as random

- Real \texttt{delta\_beta (const RealVector \&x, bool cdf\_flag, Real z\_bar)}
  return the change in reliability index (mapped from z\_bar) between two response expansions, treating a subset of variables as random

- Real \texttt{delta\_z (bool cdf\_flag, Real beta\_bar)}
  return the change in response level (mapped from beta\_bar) between two response expansions, treating all variables as random

- Real \texttt{delta\_z (const RealVector \&x, bool cdf\_flag, Real beta\_bar)}
  return the change in response level (mapped from beta\_bar) between two response expansions, treating a subset of the variables as random

- void \texttt{compute\_moments ()}
  compute moments up to the order supported by the Pecos polynomial approximation

- void \texttt{compute\_moments (const Pecos::RealVector \&x)}
  compute moments in all-variables mode up to the order supported by the Pecos polynomial approximation

- const RealVector & \texttt{moments () const}
  return virtual Pecos::PolynomialApproximation::moments()

- const RealVector & \texttt{expansion\_moments () const}
  return Pecos::PolynomialApproximation::expansionMoments

- const RealVector & \texttt{numerical\_integration\_moments () const}
  return Pecos::PolynomialApproximation::numericalMoments

- void \texttt{standardize\_moments (const Pecos::RealVector \&central\_moments, Pecos::RealVector \&std\_moments)}
  standardize the central moments returned from Pecos

- void \texttt{build\_linear\_system (RealMatrix \&A, const UShort2DArray \&multi\_index)}
  construct the Vandermonde matrix "A" for PCE regression for Ax = b
• void **augment_linear_system** (const RealVectorArray &samples, RealMatrix &A, const UShort2DArray &multi_index)
• const Pecos::SurrogateData & **surrogate_data** () const
• Pecos::BasisApproximation & **pecos_basis_approximation** ()
  
  ```
  return pecosBasisApprox
  ```

**Protected Member Functions**

• Real **value** (const Variables &vars)
  retrieve the approximate function value for a given parameter vector
• const Pecos::RealVector & **gradient** (const Variables &vars)
  retrieve the approximate function gradient for a given parameter vector
• const Pecos::RealSymMatrix & **hessian** (const Variables &vars)
  retrieve the approximate function Hessian for a given parameter vector
• int **mincoefficients** () const
  return the minimum number of samples (unknowns) required to build the derived class approximation type in num-vars dimensions
• void **build** ()
  builds the approximation from scratch
• void **rebuild** ()
  rebuilds the approximation incrementally
• void **pop** (bool save_data)
  removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args)
• void **push** ()
  restores state prior to previous pop()
• void **finalize** ()
  finalize approximation by applying all remaining trial sets
• void **store** (size_t index=NPOS)
  store current approximation state for later combination
• void **restore** (size_t index=NPOS)
  restore previous approximation state
• void **remove_stored** (size_t index=NPOS)
  remove a stored approximation prior to combination
• void **combine** (short corr_type, size_t swap_index)
  combine current approximation with previously stored approximation
• void **print_coefficients** (std::ostream &, bool normalized)
  print the coefficient array computed in build/rebuild()
• RealVector **approximation_coefficients** (bool normalized) const
  return expansion coefficients in a form consistent with the shared multi-index
• void **approximation_coefficients** (const RealVector &approx_coeffs, bool normalized)
  set expansion coefficients in a form consistent with the shared multi-index
• void **coefficient_labels** (std::vector<std::string> &coeff_labels) const
  print the coefficient array computed in build/rebuild()
Private Member Functions

- void approx\_type\_to\_basis\_type (const String &approx\_type, short &basis\_type)
  
  utility to convert Dakota type string to Pecos type enumeration

Private Attributes

- Pecos::BasisApproximation pecosBasisApprox
  
  the Pecos basis approximation, encompassing OrthogPolyApproximation and InterpPolyApproximation
- Pecos::PolynomialApproximation * polyApproxRep
  
  convenience pointer to representation of Pecos polynomial approximation

Additional Inherited Members

13.147.1 Detailed Description

Derived approximation class for global basis polynomials.

The PecosApproximation class provides a global approximation based on basis polynomials. This includes orthogonal polynomials used for polynomial chaos expansions and interpolation polynomials used for stochastic collocation.

13.147.2 Member Function Documentation

void build ( ) [inline], [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References Approximation::build(), and PecosApproximation::pecosBasisApprox.

void rebuild ( ) [inline], [protected], [virtual]

rebuilds the approximation incrementally

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References PecosApproximation::pecosBasisApprox.

void pop ( bool save\_data ) [inline], [protected], [virtual]

removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args)

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References PecosApproximation::pecosBasisApprox, and Approximation::pop().
void push ( ) [inline], [protected], [virtual]
restores state prior to previous pop()

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations
should explicitly invoke (or reimplement) this base class contribution.
Reimplemented from Approximation.
References PecosApproximation::pecosBasisApprox, and Approximation::push().

void finalize ( ) [inline], [protected], [virtual]
finalize approximation by applying all remaining trial sets

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations
should explicitly invoke (or reimplement) this base class contribution.
Reimplemented from Approximation.
References Approximation::finalize(), and PecosApproximation::pecosBasisApprox.
The documentation for this class was generated from the following files:

- PecosApproximation.hpp
- PecosApproximation.cpp

13.148 ProbabilityTransformModel Class Reference
Probability transformation specialization of RecastModel.

Inheritance diagram for ProbabilityTransformModel:

```
Model
   
RecastModel
   
ProbabilityTransformModel
```

Public Member Functions

- ProbabilityTransformModel (const Model &sub_model, bool truncated_bounds=false, Real bound=10.)
  standard constructor
- ~ProbabilityTransformModel ()
  destructor
- bool initialize_mapping (ParLevLIter pl_iter)
  initialize model mapping, returns true if the variables size has changed
- bool finalize_mapping ()
  finalize model mapping, returns true if the variables size has changed
- bool mapping_initialized () const
  return true if mapping has been fully initialized, false otherwise.
- bool resize_pending () const
  return true if a potential resize is still pending, such that sizing-based initialization should be deferred
• void transform_correlations ()
  perform correlation warping for variable types supported by Nataf

Protected Member Functions

• void distribution_parameter_derivatives (bool dist_param_derivs)
  set distParamDerivs
• void initialize_random_variables (const Pecos::ProbabilityTransformation &transform, bool deep_copy=false)
  alternate form: initialize natafTransform based on incoming data
• void initialize_random_variable_transformation ()
  instantiate natafTransform
• void initialize_random_variable_types ()
  initializes ranVarTypesX within natafTransform (u-space not needed)
• void initialize_random_variable_types (short u_space_type)
  initializes ranVarTypesX and ranVarTypesU within natafTransform
• void initialize_random_variable_parameters ()
  initializes ranVarMeansX, ranVarStdDevsX, ranVarLowerBndsX, ranVarUpperBndsX, and ranVarAddtlParamsX
  within natafTransform
• void initialize_random_variable_correlations ()
  propagate iteratedModel correlations to natafTransform
• void verify_correlation_support (short u_space_type)
  verify that correlation warping is supported by Nataf for given variable types
• void transform_model (bool truncated_bounds, Real bound)
  recast x_model from x-space to u-space to create u_model
• unsigned short pecos_to_dakota_variable_type (unsigned short pecos_var_type)
  convert from Pecos To Dakota variable enumeration type for continuous aleatory uncertain variables used in variable transformations
• void initialize_sizes ()

Static Protected Member Functions

• static void vars_u_to_x_mapping (const Variables &u_vars, Variables &x_vars)
  static function for RecastModels used for forward mapping of u-space variables from NonD Iterators to x-space variables for Model evaluations
• static void vars_x_to_u_mapping (const Variables &x_vars, Variables &u_vars)
  static function for RecastModels used for inverse mapping of x-space variables from data import to u-space variables for NonD Iterators
• static void set_u_to_x_mapping (const Variables &u_vars, const ActiveSet &u_set, ActiveSet &x_set)
  static function for RecastModels used to map u-space ActiveSets from NonD Iterators to x-space ActiveSets for Model evaluations
• static void resp_x_to_u_mapping (const Variables &x_vars, const Variables &u_vars, const Response &x_response, Response &u_response)
  static function for RecastModels used to map x-space responses from Model evaluations to u-space responses for return to NonD Iterator.
Private Attributes

- Pecos::ProbabilityTransformation natafTransform
  Nonlinear variable transformation that encapsulates the required data for performing transformations from \( X \rightarrow Z \rightarrow U \) and back.
- size_t numFunctions
  number of response functions
- size_t numContinuousVars
  number of active continuous vars
- size_t numDiscreteIntVars
  number of active discrete integer vars
- size_t numDiscreteStringVars
  number of active discrete string vars
- size_t numDiscreteRealVars
  number of active discrete real vars
- size_t numContDesVars
  number of continuous design variables (modeled using uniform distribution for All view modes)
- size_t numDiscIntDesVars
  number of discrete integer design variables (modeled using discrete histogram distributions for All view modes)
- size_t numDiscStringDesVars
  number of discrete string design variables (modeled using discrete histogram distributions for All view modes)
- size_t numDiscRealDesVars
  number of discrete real design variables (modeled using discrete histogram distributions for All view modes)
- size_t numDesignVars
  total number of design variables
- size_t numContStateVars
  number of continuous state variables (modeled using uniform distribution for All view modes)
- size_t numDiscIntStateVars
  number of discrete integer state variables (modeled using discrete histogram distributions for All view modes)
- size_t numDiscStringStateVars
  number of discrete string state variables (modeled using discrete histogram distributions for All view modes)
- size_t numDiscRealStateVars
  number of discrete real state variables (modeled using discrete histogram distributions for All view modes)
- size_t numStateVars
  total number of state variables
- size_t numNormalVars
  number of normal uncertain variables (native space)
- size_t numLognormalVars
  number of lognormal uncertain variables (native space)
- size_t numUniformVars
  number of uniform uncertain variables (native space)
- size_t numLoguniformVars
  number of loguniform uncertain variables (native space)
- size_t numTriangularVars
number of triangular uncertain variables (native space)

- size_t numExponentialVars
  number of exponential uncertain variables (native space)

- size_t numBetaVars
  number of beta uncertain variables (native space)

- size_t numGammaVars
  number of gamma uncertain variables (native space)

- size_t numGumbelVars
  number of gumbel uncertain variables (native space)

- size_t numFrechetVars
  number of frechet uncertain variables (native space)

- size_t numWeibullVars
  number of weibull uncertain variables (native space)

- size_t numHistogramBinVars
  number of histogram bin uncertain variables (native space)

- size_t numPoissonVars
  number of Poisson uncertain variables (native space)

- size_t numBinomialVars
  number of binomial uncertain variables (native space)

- size_t numNegBinomialVars
  number of negative binomial uncertain variables (native space)

- size_t numGeometricVars
  number of geometric uncertain variables (native space)

- size_t numHyperGeomVars
  number of hypergeometric uncertain variables (native space)

- size_t numHistogramPtIntVars
  number of histogram point integer uncertain variables (native space)

- size_t numHistogramPtStringVars
  number of histogram point string uncertain variables (native space)

- size_t numHistogramPtRealVars
  number of histogram point real uncertain variables (native space)

- size_t numContIntervalVars
  number of continuous interval uncertain variables (native space)

- size_t numDiscIntervalVars
  number of discrete interval uncertain variables (native space)

- size_t numDiscSetIntUncVars
  number of discrete integer set uncertain variables (native space)

- size_t numDiscSetStringUncVars
  number of discrete integer set uncertain variables (native space)

- size_t numDiscSetRealUncVars
  number of discrete real set uncertain variables (native space)

- size_t numContAleatUncVars
  total number of continuous aleatory uncertain variables (native space)
• `size_t numDiscIntAleatUncVars`
  total number of discrete integer aleatory uncertain variables (native space)

• `size_t numDiscStringAleatUncVars`
  total number of discrete string aleatory uncertain variables (native space)

• `size_t numDiscRealAleatUncVars`
  total number of discrete real aleatory uncertain variables (native space)

• `size_t numAleatoryUncVars`
  total number of aleatory uncertain variables (native space)

• `size_t numContEpistUncVars`
  total number of continuous epistemic uncertain variables (native space)

• `size_t numDiscIntEpistUncVars`
  total number of discrete integer epistemic uncertain variables (native space)

• `size_t numDiscStringEpistUncVars`
  total number of discrete string epistemic uncertain variables (native space)

• `size_t numDiscRealEpistUncVars`
  total number of discrete real epistemic uncertain variables (native space)

• `size_t numEpistemicUncVars`
  total number of epistemic uncertain variables (native space)

• `size_t numUncertainVars`
  total number of uncertain variables (native space)

• `bool distParamDerivs`
  flags calculation of derivatives with respect to distribution parameters s within `resp_x_to_u_mapping()` using the chain rule df/dx dx/ds. The default is to calculate derivatives with respect to standard random variables u using the chain rule df/dx dx/du.

• `bool truncatedBounds`
  boolean flag to indicate truncated bounds

• `Real boundVal`
  bound value

• `bool epistemicStats`
  flag for computing interval-type metrics instead of integrated metrics If any epistemic variables are active in a metric evaluation, then this flag is set.

• `SizetArray primaryACVarMapIndices`
  "primary" all continuous variable mapping indices flowed down from higher level iteration

• `ShortArray secondaryACVarMapTargets`
  "secondary" all continuous variable mapping targets flowed down from higher level iteration

• `bool mappingInitialized`
  track use of `initialize_mapping()` and `finalize_mapping()`

Static Private Attributes

• `static ProbabilityTransformModel * ptmInstance`
  static pointer to this class for use in static callbacks
Additional Inherited Members

13.148.1 Detailed Description

Probability transformation specialization of RecastModel.

Specialization of RecastModel to transform a sub-model to u-space.

13.148.2 Member Function Documentation

**void initialize_random_variables ( const Pecos::ProbabilityTransformation & transform, bool deep_copy = false ) [protected]**

alternate form: initialize natafTransform based on incoming data

This function is commonly used to publish transformation data when the Model variables are in a transformed space (e.g., u-space) and ProbabilityTransformation::ranVarTypes et al. may not be generated directly. This allows for the use of inverse transformations to return the transformed space variables to their original states.

References ProbabilityTransformModel::initialize_random_variable_transformation(), ProbabilityTransformModel::natafTransform, ProbabilityTransformModel::numContDesVars, ProbabilityTransformModel::numContEpistUncVars, ProbabilityTransformModel::numContIntervalVars, and ProbabilityTransformModel::numContStateVars.

**void initialize_random_variable_types ( ) [protected]**

initializes ranVarTypesX within natafTransform (u-space not needed)

Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.


Referenced by ProbabilityTransformModel::ProbabilityTransformModel().

**void initialize_random_variable_types ( short u_space_type ) [protected]**

initializes ranVarTypesX and ranVarTypesU within natafTransform

Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.

References Dakota::abort_handler(), Model::aleatory_distribution_parameters(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), ProbabilityTransformModel::natafTransform, ProbabilityTransformModel::numBetaVars, ProbabilityTransformModel::numBinomialVars, ProbabilityTransformModel::numContDesVars, ProbabilityTransformModel::numContIntervalVars, ProbabilityTransformModel::numContStateVars, ProbabilityTransformModel::numExponentialVars, ProbabilityTransformModel::numFrechetVars, ProbabilityTransformModel::numGammaVars, ProbabilityTransformModel::numGeometricVars, ProbabilityTransformModel::numGumbelVars, ProbabilityTransformModel::numNormalVars, ProbabilityTransformModel::numPoissonVars, ProbabilityTransformModel::numTriangularVars, ProbabilityTransformModel::numUniformVars, ProbabilityTransformModel::numWeibullVars, and RecastModel::subModel.
BinomialVars, ProbabilityTransformModel::numNormalVars, ProbabilityTransformModel::numPoissonVars, ProbabilityTransformModel::numTriangularVars, ProbabilityTransformModel::numUniformVars, ProbabilityTransformModel::numWeibullVars, and RecastModel::subModel.

void initialize_random_variable_parameters() [protected]
initializes ranVarMeansX, ranVarStdDevsX, ranVarLowerBndsX, ranVarUpperBndsX, and ranVarAddtlParamsX within natafTransform
Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.
References Model::aleatory_distribution_parameters(), Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::epistemic_distribution_parameters(), ProbabilityTransformModel::natafTransform, ProbabilityTransformModel::numAleatoryUncVars, ProbabilityTransformModel::numContDesVars, ProbabilityTransformModel::numContinuousVars, ProbabilityTransformModel::numContStateVars, ProbabilityTransformModel::numEpistemicUncVars, and RecastModel::subModel.
Referenced by ProbabilityTransformModel::initialize_mapping().

void vars_u_to_x_mapping ( const Variables & u_vars, Variables & x_vars ) [inline], [static], [protected]
static function for RecastModels used for forward mapping of u-space variables from NonD Iterators to x-space variables for Model evaluations
Map the variables from iterator space (u) to simulation space (x).
References Variables::continuous_variables(), Variables::continuous_variables_view(), ProbabilityTransformModel::natafTransform, and ProbabilityTransformModel::ptmInstance.
Referenced by ProbabilityTransformModel::ProbabilityTransformModel().

void vars_x_to_u_mapping ( const Variables & x_vars, Variables & u_vars ) [inline], [static], [protected]
static function for RecastModels used for inverse mapping of x-space variables from data import to u-space variables for NonD Iterators
Map the variables from simulation space (x) to iterator space (u).
References Variables::continuous_variables(), Variables::continuous_variables_view(), ProbabilityTransformModel::natafTransform, and ProbabilityTransformModel::ptmInstance.
Referenced by ProbabilityTransformModel::ProbabilityTransformModel().

void set_u_to_x_mapping ( const Variables & u_vars, const ActiveSet & u_set, ActiveSet & x_set ) [static], [protected]
static function for RecastModels used to map u-space ActiveSets from NonD Iterators to x-space ActiveSets for Model evaluations
Define the DVV for x-space derivative evaluations by augmenting the iterator requests to account for correlations.
References Dakota::NPOS, Variables::all_continuous_variable_ids(), Dakota::contains(), Variables::continuous_variable_ids(), ActiveSet::derivative_vector(), Dakota::find_index(), Variables::inactive_continuous_variable_ids(), ProbabilityTransformModel::natafTransform, and ProbabilityTransformModel::ptmInstance.
Referenced by ProbabilityTransformModel::ProbabilityTransformModel().
13.148.3 Member Data Documentation

**ProbabilityTransformModel** 

Member **ptmInstance**  

- static
- [static], [private]

Static pointer to this class for use in static callbacks  
initialization of static needed by **RecastModel**

Referenced by **ProbabilityTransformModel::ProbabilityTransformModel()**, **ProbabilityTransformModel::resp_x_to_u_mapping()**, **ProbabilityTransformModel::set_u_to_x_mapping()**, **ProbabilityTransformModel::vars_u_to_x_mapping()**, and **ProbabilityTransformModel::vars_x_to_u_mapping()**.  
The documentation for this class was generated from the following files:

- ProbabilityTransformModel.hpp  
- ProbabilityTransformModel.cpp

13.149 ProblemDescDB Class Reference

The database containing information parsed from the DAKOTA input file.

Inheritance diagram for ProblemDescDB:

```
ProblemDescDB  
\downarrow  
NIDRProblemDescDB
```

### Public Member Functions

- **ProblemDescDB ()**  
  default constructor

- **ProblemDescDB (ParallelLibrary &parallel_lib)**  
  standard constructor

- **ProblemDescDB (const ProblemDescDB &db)**  
  copy constructor

- **~ProblemDescDB ()**  
  destructor

- **ProblemDescDB operator= (const ProblemDescDB &db)**  
  assignment operator

- **void parse_inputs (const ProgramOptions &prog_opts, DbCallbackFunctionPtr callback=NULL, void *callback_data=NULL)**

  Parses the input file or input string if present and executes callbacks. Does not perform any validation.

- **void check_and_broadcast (const ProgramOptions &prog_opts)**

  Performs check_input, broadcast, and post_process, but for now, allowing separate invocation through the public API as well

- **void check_input ()**

  Verifies that there is at least one of each of the required keywords in the dakota input file

- **void broadcast ()**
invokes send_db_buffer() and receive_db_buffer() to broadcast DB data across the processor allocation. Used by manage_inputs().

- void post_process()
  post-processes the (minimal) input specification to assign default variables/responses specification arrays. Used by manage_inputs().

- void lock()
  Locks the database in order to prevent data access when the list nodes may not be set properly. Unlocked by a set nodes operation.

- void unlock()
  Explicitly unlocks the database. Use with care.

- void set_db_list_nodes (const String &method_tag)
  set dataMethodIter based on a method identifier string to activate a particular method specification in dataMethodList and use pointers from this method specification to set all other list iterators.

- void set_db_list_nodes (size_t method_index)
  set dataMethodIter based on an index within dataMethodList to activate a particular method specification and use pointers from this method specification to set all other list iterators.

- void resolve_top_method (bool set_model_nodes=true)
  For a (default) environment lacking a top method pointer, this function is used to determine which of several potential method specifications corresponds to the top method and then sets the list nodes accordingly.

- void set_db_method_node (const String &method_tag)
  set dataMethodIter based on a method identifier string to activate a particular method specification (only).

- void set_db_method_node (size_t method_index)
  set dataMethodIter based on an index within dataMethodList to activate a particular method specification (only).

- size_t get_db_method_node()
  return the index of the active node in dataMethodList

- void set_db_model_nodes (const String &model_tag)
  set the model list iterators (dataModelIter, dataVariablesIter, dataInterfaceIter, and dataResponsesIter) based on the model identifier string

- void set_db_model_nodes (size_t model_index)
  set the model list iterators (dataModelIter, dataVariablesIter, dataInterfaceIter, and dataResponsesIter) based on an index within dataModelList

- size_t get_db_model_node()
  return the index of the active node in dataModelList

- void set_db_variables_node (const String &variables_tag)
  set dataVariablesIter based on the variables identifier string

- void set_db_interface_node (const String &interface_tag)
  set dataInterfaceIter based on the interface identifier string

- void set_db_responses_node (const String &responses_tag)
  set dataResponsesIter based on the responses identifier string

- ParallelLibrary & parallel_library () const
  return the parallelLib reference

- IteratorList & iterator_list () const
  return a list of all Iterator objects that have been instantiated

- ModelList & model_list ()
  return a list of all Model objects that have been instantiated
- VariablesList & variables_list ()
  return a list of all Variables objects that have been instantiated
- InterfaceList & interface_list ()
  return a list of all Interface objects that have been instantiated
- ResponseList & response_list ()
  return a list of all Response objects that have been instantiated
- const RealMatrixArray & get_rma (const String &entry_name) const
  get a RealMatrixArray out of the database based on an identifier string
- const RealVector & get(rv) (const String &entry_name) const
  get a RealVector out of the database based on an identifier string
- const IntVector & get_iv (const String &entry_name) const
  get an IntVector out of the database based on an identifier string
- const BitArray & get ba (const String &entry_name) const
  get a BitArray out of the database based on an identifier string
- const SizetArray & get_sza (const String &entry_name) const
  get a SizetArray out of the database based on an identifier string
- const UShortArray & get_usa (const String &entry_name) const
  get a UShortArray out of the database based on an identifier string
- const RealSymMatrix & get_rsm (const String &entry_name) const
  get a RealSymMatrix out of the database based on an identifier string
- const RealVectorArray & get_rva (const String &entry_name) const
  get a RealVectorArray out of the database based on an identifier string
- const IntVectorArray & get_jva (const String &entry_name) const
  get an IntVectorArray out of the database based on an identifier string
- const IntSet & get_is (const String &entry_name) const
  get an IntSet out of the database based on an identifier string
- const IntSetArray & get_isa (const String &entry_name) const
  get an IntSetArray out of the database based on an identifier string
- const StringSetArray & get_ssa (const String &entry_name) const
  get a StringSetArray out of the database based on an identifier string
- const RealSetArray & get_rsa (const String &entry_name) const
  get a RealSetArray out of the database based on an identifier string
- const IntRealMapArray & get_irma (const String &entry_name) const
  get an IntRealMapArray out of the database based on an identifier string
- const StringRealMapArray & get_srm (const String &entry_name) const
  get a StringRealMapArray out of the database based on an identifier string
- const RealRealMapArray & get_rma (const String &entry_name) const
  get a RealRealMapArray out of the database based on an identifier string
- const RealRealPairRealMapArray & get_rrma (const String &entry_name) const
  get a RealRealPairRealMapArray out of the database based on an identifier string
- const IntIntPairRealMapArray & get_irma (const String &entry_name) const
  get an IntIntPairRealMapArray out of the database based on an identifier string
- const StringArray & get_sa (const String &entry_name) const
get a StringArray out of the database based on an identifier string

- const String2DArray & get_s2a (const String &entry_name) const
  get a String2DArray out of the database based on an identifier string
- const String & get_string (const String &entry_name) const
  get a String out of the database based on an identifier string
- const Real & get_real (const String &entry_name) const
  get a Real out of the database based on an identifier string
- int get_int (const String &entry_name) const
  get an int out of the database based on an identifier string
- short get_short (const String &entry_name) const
  get a short out of the database based on an identifier string
- unsigned short get_ushort (const String &entry_name) const
  get an unsigned short out of the database based on an identifier string
- size_t get_sizet (const String &entry_name) const
  get a size_t out of the database based on an identifier string
- bool get_bool (const String &entry_name) const
  get a bool out of the database based on an identifier string
- void ** get_voidss (const String &entry_name) const
  for getting a void**, e.g., &dlLib
- void insert_node (const DataEnvironment &data_env)
  set the DataEnvironment object
- void insert_node (const DataMethod &data_method)
  add a DataMethod object to the dataMethodList
- void insert_node (const DataModel &data_model)
  add a DataModel object to the dataModelList
- void insert_node (DataVariables &data_variables)
  add a DataVariables object to the dataVariablesList
- void insert_node (const DataInterface &data_interface)
  add a DataInterface object to the dataInterfaceList
- void insert_node (const DataResponses &data_responses)
  add a DataResponses object to the dataResponsesList
- void set (const String &entry_name, const RealVector &rv)
  set a RealVector within the database based on an identifier string
- void set (const String &entry_name, const IntVector &iv)
  set an IntVector within the database based on an identifier string
- void set (const String &entry_name, const BitArray &ba)
  set a BitArray within the database based on an identifier string
- void set (const String &entry_name, const RealSymMatrix &rsm)
  set a RealMatrix within the database based on an identifier string
- void set (const String &entry_name, const RealVectorArray &rva)
  set a RealVectorArray within the database based on an identifier string
- void set (const String &entry_name, const IntVectorArray &iva)
  set an IntVectorArray within the database based on an identifier string
• void set (const String &entry_name, const IntSetArray &isa)
  set an IntSetArray within the database based on an identifier string
• void set (const String &entry_name, const RealSetArray &rsa)
  set a RealSetArray within the database based on an identifier string
• void set (const String &entry_name, const IntRealMapArray &irma)
  set an IntRealMapArray within the database based on an identifier string
• void set (const String &entry_name, const StringRealMapArray &srma)
  set a StringRealMapArray within the database based on an identifier string
• void set (const String &entry_name, const RealRealMapArray &rrma)
  set a RealRealMapArray within the database based on an identifier string
• void set (const String &entry_name, const RealRealPairRealMapArray &iirma)
  set a RealRealPairRealMapArray in the db based on an identifier string
• void set (const String &entry_name, const IntIntPairRealMapArray &iirma)
  set an IntIntPairRealMapArray in the db based on an identifier string
• void set (const String &entry_name, const StringArray &sa)
  set a StringArray within the database based on an identifier string
• int min_procs_per_ea ()
  compute minimum evaluation partition size based on lower level overrides
• int max_procs_per_ea ()
  compute maximum evaluation partition size based on lower level overrides and concurrency levels
• int min_procs_per_ie ()
  compute minimum iterator partition size based on lower level overrides
• int max_procs_per_ie (int max_eval_concurrency)
  compute maximum iterator partition size based on lower level overrides and concurrency levels
• bool method_locked () const
  return methodDBLocked
• bool model_locked () const
  return modelDBLocked
• bool variables_locked () const
  return variablesDBLocked
• bool interface_locked () const
  return interfaceDBLocked
• bool responses_locked () const
  return responsesDBLocked
• bool is_null () const
  function to check dbRep (does this envelope contain a letter)

Static Public Member Functions

• static int min_procs_per_level (int min_procs_per_server, int pps_spec, int num_serv_spec)
  compute minimum partition size for a parallel level based on lower level overrides
• static int max_procs_per_level (int max_procs_per_server, int pps_spec, int num_serv_spec, short sched_spec,
  int asyncr_local_conc, bool peer_dynamic_avail, int max_concurrency)
  compute maximum partition size for a parallel level based on lower level overrides
Protected Member Functions

- **ProblemDescDB** (*BaseConstructor*, `ParallelLibrary` & `parallel_lib`)
  
  *constructor initializes the base class part of letter classes* (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

- virtual void **derived_parse_inputs** (const `ProgramOptions` & `prog_opts`)
  
  *derived class specifics within parse_inputs()*

- virtual void **derived_broadcast** ()
  
  *derived class specifics within broadcast()*

- virtual void **derived_post_process** ()
  
  *derived class specifics within post_process()*

Protected Attributes

- **DataEnvironment** `environmentSpec`
  
  *the environment specification (only one allowed) resulting from a call to environment_kwhandler() or insert_node()*

- std::list< `DataMethod` > `dataMethodList`
  
  *list of method specifications, one for each call to method_kwhandler() or insert_node()*

- std::list< `DataModel` > `dataModelList`
  
  *list of model specifications, one for each call to model_kwhandler() or insert_node()*

- std::list< `DataVariables` > `dataVariablesList`
  
  *list of variables specifications, one for each call to variables_kwhandler() or insert_node()*

- std::list< `DataInterface` > `dataInterfaceList`
  
  *list of interface specifications, one for each call to interface_kwhandler() or insert_node()*

- std::list< `DataResponses` > `dataResponsesList`
  
  *list of responses specifications, one for each call to responses_kwhandler() or insert_node()*

- size_t **environmentCntr**
  
  *counter for environment specifications used in check_input*

Private Member Functions

- const **Iterator & get_iterator** ()
  
  *retrieve an existing w itor, if it exists in iteratorList, or instantiate a new one*

- const **Iterator & get_iterator** (Model & `model`)
  
  *retrieve an existing Iterator, if it exists in iteratorList, or instantiate a new one*

- const **Iterator & get_iterator** (const String & `method_name`, Model & `model`)
  
  *retrieve an existing Iterator, if it exists in iteratorByNameList, or instantiate a new one*

- const **Model & get_model** ()
  
  *retrieve an existing Model, if it exists, or instantiate a new one*

- const **Variables & get_variables** ()
  
  *retrieve an existing Variables, if it exists, or instantiate a new one*

- const **Interface & get_interface** ()
  
  *retrieve an existing Interface, if it exists, or instantiate a new one*

- const **Response & get_response** (short type, const Variables & `vars`)
  
  *retrieve an existing Response, if it exists, or instantiate a new one*
• ProblemDescDB * get_db (ParallelLibrary &parallel_lib)
  
  Used by the envelope constructor to instantiate the correct letter class.
• void send_db_buffer ()
  
  MPI send of a large buffer containing environmentSpec and all objects in dataMethodList, dataModelList, dataVariablesList, dataInterfaceList, and dataResponsesList. Used by manage_inputs().
• void receive_db_buffer ()
  
  MPI receive of a large buffer containing environmentSpec and all objects in dataMethodList, dataModelList, dataVariablesList, dataInterfaceList, and dataResponsesList. Used by manage_inputs().
• bool model_has_interface (DataModelRep *model_rep) const
  
  helper function for determining whether an interface specification should be active, based on model type
• void echo_input_file (const ProgramOptions &prog_opts)
  
  echo the (potentially) specified input file or string to stdout

Private Attributes

• ParallelLibrary & parallelLib
  
  reference to the parallel_lib object passed from main
• std::list< DataMethod >::iterator dataMethodIter
  
  iterator identifying the active list node in dataMethodList
• std::list< DataModel >::iterator dataModelIter
  
  iterator identifying the active list node in dataModelList
• std::list< DataVariables >::iterator dataVariablesIter
  
  iterator identifying the active list node in dataVariablesList
• std::list< DataInterface >::iterator dataInterfaceIter
  
  iterator identifying the active list node in dataInterfaceList
• std::list< DataResponses >::iterator dataResponsesIter
  
  iterator identifying the active list node in dataResponsesList
• IteratorList iteratorList
  
  list of iterator objects, one for each method specification
• IteratorList iteratorByNameList
  
  list of iterator objects, one for each lightweight instantiation by name
• ModelList modelList
  
  list of model objects, one for each model specification
• VariablesList variablesList
  
  list of variables objects, one for each variables specification
• InterfaceList interfaceList
  
  list of interface objects, one for each interface specification
• ResponseList responseList
  
  list of response objects, one for each responses specification
• bool methodDBLocked
  
  prevents use of get_<type> retrieval and set_<type> update functions prior to setting the list node for the active method specification
• bool modelDBLocked
  prevents use of get_{<type>} retrieval and set_{<type>} update functions prior to setting the list node for the active model specification
• bool variablesDBLocked
  prevents use of get_{<type>} retrieval and set_{<type>} update functions prior to setting the list node for the active variables specification
• bool interfaceDBLocked
  prevents use of get_{<type>} retrieval and set_{<type>} update functions prior to setting the list node for the active interface specification
• bool responsesDBLocked
  prevents use of get_{<type>} retrieval and set_{<type>} update functions prior to setting the list node for the active responses specification
• ProblemDesc * dbRep
  pointer to the letter (initialized only for the envelope)
• int referenceCount
  number of objects sharing dbRep

Friends

• class Model
  Model requires access to get_variables() and get_response()
• class SimulationModel
  SimulationModel requires access to get_interface()
• class HierarchSurrModel
  HierarchSurrModel requires access to get_model()
• class DataFitSurrModel
  DataFitSurrModel requires access to get Iterator() and get_model()
• class NestedModel
  NestedModel requires access to get_interface(), get_response(), get_iterator(), and get_model()
• class ActiveSubspaceModel
• class AdaptedBasisModel
• class RandomFieldModel
• class Environment
  Environment requires access to get_iterator()
• class IteratorScheduler
  Environment requires access to get_iterator()
• class Iterator
  Iterator requires access to get_model()
• class MetaIterator
  Iterator requires access to get_model()
• class SeqHybridMetaIterator
  SeqHybridMetaIterator requires access to get_model()
• class CollabHybridMetaIterator
  CollabHybridMetaIterator requires access to get_model()
• class ConcurrentMetaIterator
  
  ConcurrentMetaIterator requires access to get_model()

• class SurrBasedLocalMinimizer
  
  HierarchSurrBasedLocalMinimizer requires access to get_iterator()

• class SurrBasedGlobalMinimizer
  
  SurrBasedGlobalMinimizer requires access to get_iterator()

• class PebbldMinimizer
  
  PEBBLMinimizer requires access to get_iterator()

13.149.1 Detailed Description

The database containing information parsed from the DAKOTA input file.

The ProblemDescDB class is a database for DAKOTA input file data that is populated by a parser defined in a derived class. When the parser reads a complete keyword, it populates a data class object (DataEnvironment, DataMethod, DataVariables, DataInterface, or DataResponses) and, for all cases except environment, appends the object to a linked list (dataMethodList, dataVariablesList, dataInterfaceList, or dataResponsesList). No environment linked list is used since only one environment specification is allowed.

13.149.2 Constructor & Destructor Documentation

ProblemDescDB ( )

default constructor

  The default constructor: dbRep is NULL in this case. This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

ProblemDescDB ( ParallelLibrary & parallel_lib )

standard constructor

  This is the envelope constructor which uses problem_db to build a fully populated db object. It only needs to extract enough data to properly execute get_db(problem_db), since the constructor overloaded with BaseConstructor builds the actual base class data inherited by the derived classes.

  References Dakota::abort_handler(), ProblemDescDB::dbRep, and ProblemDescDB::get_db().

ProblemDescDB ( const ProblemDescDB & db )

copy constructor

  Copy constructor manages sharing of dbRep and incrementing of referenceCount.

  References ProblemDescDB::dbRep, and ProblemDescDB::referenceCount.

~ProblemDescDB ( )

destructor

  Destructor decrements referenceCount and only deletes dbRep when referenceCount reaches zero.

  References Dakota::Dak_pddb, ProblemDescDB::dbRep, and ProblemDescDB::referenceCount.
ProblemDescDB ( BaseConstructor, ParallelLibrary & parallel_lib ) [protected]

class constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_db() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid the recursion of the base class constructor calling get_db() again). Since the letter IS the representation, its representation pointer is set to NULL (an uninitialized pointer causes problems in ~ProblemDescDB).

13.149.3 Member Function Documentation

ProblemDescDB operator= ( const ProblemDescDB & db )

assignment operator


References ProblemDescDB::dbRep, and ProblemDescDB::referenceCount.

void parse_inputs ( const ProgramOptions & prog_opts, DbCallbackFunctionPtr callback = NULL, void * callback_data = NULL )

Parses the input file or input string if present and executes callbacks. Does not perform any validation.

DB setup phase 1: parse the input file and execute callback functions if present. Rank 0 only.

DB setup phase 2: optionally insert additional data via late sets. Rank 0 only.

References Dakota::abort_handler(), ProblemDescDB::dbRep, ProblemDescDB::derived_parse_inputs(), ProgramOptions::echo_input(), ProblemDescDB::echo_input_file(), ProgramOptions::input_file(), ProgramOptions::input_string(), ProblemDescDB::parallelLib, ProblemDescDB::parse_inputs(), and ParallelLibrary::world_rank().

Referenced by Environment::parse(), and ProblemDescDB::parse_inputs().

void check_and_broadcast ( const ProgramOptions & prog_opts )

performs check_input, broadcast, and post_process, but for now, allowing separate invocation through the public API as well

DB setup phase 3: perform basic checks on keywords counts in current DB state, then sync to all processors.

References ProblemDescDB::broadcast(), ProblemDescDB::check_and_broadcast(), ProblemDescDB::check_input(), ProblemDescDB::dbRep, ProblemDescDB::parallelLib, ProblemDescDB::post_process(), and ParallelLibrary::world_rank().

Referenced by ProblemDescDB::check_and_broadcast(), LibraryEnvironment::done_modifying_db(), and Environment::parse().

void check_input ( )

verifies that there is at least one of each of the required keywords in the dakota input file

NOTE: when using library mode in a parallel application, check_input() should either be called only on world-Rank 0, or it should follow a matched send_db_buffer()/receive_db_buffer() pair.

References Dakota::abort_handler(), ProblemDescDB::check_input(), ParallelLibrary::command_line_post_run_input(), ParallelLibrary::command_line_post_run_output(), ParallelLibrary::command_line_pre_run_input(), ParallelLibrary::command_line_pre_run_output(), ParallelLibrary::command_line_run_input(), ParallelLibrary::command_line_run_output(), ParallelLibrary::command_line_user_modes(), ProblemDescDB::dataInterfaceList, ProblemDescDB::dataMethodList, ProblemDescDB::dataModelList, ProblemDescDB::dataResponsesList, ProblemDescDB::data…
CHAPTER 13. CLASS DOCUMENTATION

::dataVariablesList, ProblemDescDB::dbRep, ProblemDescDB::environmentCntr, ProblemDescDB::parallelLib, and Dakota::strbegins().

Referenced by ProblemDescDB::check_and_broadcast(), and ProblemDescDB::check_input().

```cpp
void post_process()
```

post-processes the (minimal) input specification to assign default variables/responses specification arrays. Used by manage_inputs().

When using library mode in a parallel application, post_process() should be called on all processors following broadcast() of a minimal problem specification.

References ProblemDescDB::dbRep, and ProblemDescDB::derived_post_process().

Referenced by ProblemDescDB::check_and_broadcast().

```cpp
ProblemDescDB * get_db( ParallelLibrary & parallel_lib ) [private]
```

Used by the envelope constructor to instantiate the correct letter class.

Initializes dbRep to the appropriate derived type. The standard derived class constructors are invoked.

References Dakota::Dak_pddb.

Referenced by ProblemDescDB::ProblemDescDB().

The documentation for this class was generated from the following files:

- ProblemDescDB.hpp
- ProblemDescDB.cpp

13.150 ProcessApplicInterface Class Reference

Derived application interface class that spawns a simulation code using a separate process and communicates with it through files.

Inheritance diagram for ProcessApplicInterface:

```
        Interface
         |     |
         |     |
        ApplicationInterface
         |     |
        ProcessApplicInterface
         |     |
        ProcessHandleApplicInterface      SysCallApplicInterface
         |     |
        ForkApplicInterface      SpawnApplicInterface      GridApplicInterface
```

Public Member Functions

- ProcessApplicInterface (const ProblemDescDB &problem_db)

  constructor

- ~ProcessApplicInterface ()

  destructor
13.150. PROCESSAPPLICINTERFACE CLASS REFERENCE

Protected Member Functions

- **void derived_map** (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)
  
  Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.

- **void derived_map_asynch** (const ParamResponsePair &pair)
  
  Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.

- **const StringArray & analysis_drivers () const**
  
  retrieve the analysis drivers specification for application interfaces

- **void file_cleanup () const**

- **void remove_params_results_files** (const bfs::path &params_path, const bfs::path &results_path) const
  
  Remove (potentially autotagged for multiple programs) parameters and results files with passed root names.

- **void autotag_files** (const bfs::path &params_path, const bfs::path &results_path, const String &eval_id_tag) const
  
  Utility to automatically tag parameters and results files with passed root names (the files may already need per-program tagging)

- **virtual void map_bookkeeping** (pid_t pid, int fn_eval_id)=0
  
  bookkeeping of process and evaluation ids for asynchronous maps

- **virtual pid_t create_evaluation_process** (bool block_flag)=0
  
  Spawn the evaluation by managing the input filter, analysis drivers, and output filter. Called from derived_map() & derived_map_asynch().

- **void synchronous_local_analyses** (int start, int end, int step)
  
  execute analyses synchronously on the local processor

- **void define_filenames** (const String &eval_id_tag)
  
  define modified filenames from user input by handling Unix temp file and optionally tagging with given eval_id_tag

- **void write_parameters_files** (const Variables &vars, const ActiveSet &set, const Response &response, const int id)
  
  write the parameters data and response request data to one or more parameters files (using one or more invocations of write_parameters_file()) in either standard or aprepro format

- **void read_results_files** (Response &response, const int id, const String &eval_id_tag)
  
  read the response object from one or more results files using full eval_id_tag passed

- **bfs::path get_workdir_name ()**
  
  construct a work directory name (tmp or named), with optional tag

- **void prepare_process_environment ()**
  
  set PATH, environment variables, and change directory prior to fork/system/spawn

- **void reset_process_environment ()**
  
  reset PATH and current directory after system/spawn (workdir case)

Protected Attributes

- **bool fileTagFlag**
  
  flags tagging of parameter/results files

- **bool fileSaveFlag**
  
  flags retention of parameter/results files
- **bool** `commandLineArgs`
  
  flag indicating use of passing of filenames as command line arguments to the analysis drivers and input/output filters

- **bool** `apreproFlag`
  
  flag indicating use of the APREPRO (the Sandia "A PRE PROcessor" utility) format for parameter files

- **unsigned short** `resultsFileFormat`
  
  results file format

- **bool** `multipleParamsFiles`
  
  flag indicating the need for separate parameters files for multiple analysis drivers

- **std::string** `iFilterName`
  
  the name of the input filter (input filter user specification)

- **std::string** `oFilterName`
  
  the name of the output filter (output filter user specification)

- **std::vector<String>** `programNames`
  
  the names of the analysis code programs (analysis drivers user specification)

- **std::string** `specifiedParamsFileName`
  
  the name of the parameters file from user specification

- **std::string** `paramsFileName`
  
  the parameters file name actually used (modified with tagging or temp files); only valid from define filenames to write parameters files

- **std::string** `paramsFileWritten`
  
  actual, qualified name of the params file written, possibly with workdir

- **std::string** `specifiedResultsFileName`
  
  the name of the results file from user specification

- **std::string** `resultsFileName`
  
  the results file name actually used (modified with tagging or temp files); only valid from define filenames to write parameters files

- **std::string** `resultsFileWritten`
  
  actual, qualified name of the results file written, possibly with workdir

- **std::string** `fullEvalId`
  
  complete evalIdTag, possibly including hierarchical tagging and final eval id, but not program numbers, for passing to write parameters files

- **bool** `allowExistingResults`
  
  by default analysis code interfaces delete results files if they exist; user may override with this flag and we’ll try to gather and only fork if needed

- **std::map<int, PathTriple>** `fileNameMap`
  
  Maps function evaluation ID to triples (parameters, results, and workdir) paths used in spawning function evaluations. Workdir will be empty if not created specifically for this eval.

- **bool** `useWorkdir`
  
  whether to use a work directory

- **std::string** `workDirName`
  
  work directory name, if specified...

- **bool** `dirTag`
  
  whether to tag the working directory
13.150. PROCESSAPPLICINTERFACE CLASS REFERENCE

- **bool dirSave**
  
  whether dir_save was specified

- **bfs::path curWorkdir**
  
  active working directory for this evaluation; valid only from define_filenames to create_evaluation_process

- **bfs::path createdDir**
  
  non-empty if created for this eval; valid only from define_filenames to write_parameters_files

- **StringArray linkFiles**
  
  template directory (if specified)

- **StringArray copyFiles**
  
  template files (if specified)

- **bool templateReplace**
  
  whether to replace existing files

**Private Member Functions**

- **void write_parameters_file** (const Variables &vars, const ActiveSet &set, const Response &response, const std::string &prog, const std::vector<String> &an_comps, const std::string &params_fname)

  write the variables, active set vector, derivative variables vector, and analysis components to the specified parameters file in either standard or aprepro format

- **void read_results_file** (Response &response, const bfs::path &path, const int id)

  Open and read the results file at path, properly handling errors.

**Private Attributes**

- **String2DArray analysisComponents**

  the set of optional analysis components used by the analysis drivers (from the analysis_components interface specification)

13.150.1 Detailed Description

Derived application interface class that spawns a simulation code using a separate process and communicates with it through files.

**ProcessApplicInterface** is subclassed for process handles or file completion testing.

13.150.2 Member Function Documentation

**void file_cleanup** ( ) const [protected], [virtual]

Remove any files and directories still referenced in the fileNameMap

Reimplemented from **Interface**.

References WorkdirHelper::concat_path(), ProcessApplicInterface::dirSave, ProcessApplicInterface::fileNameMap, ProcessApplicInterface::fileSaveFlag, ProcessApplicInterface::iFilterName, ProcessApplicInterface::multipleParamsFiles, ProcessApplicInterface::programNames, and WorkdirHelper::recursive_remove().
void autotag\_files (const bfs::path & params\_path, const bfs::path & results\_path, const String & eval\_id\_tag ) const [protected]

Utility to automatically tag parameters and results files with passed root names (the files may already need preprogram tagging)

Move specified params and results files to unique tagged versions when needed

References WorkdirHelper::concat\_path(), ProcessApplicInterface::FilterName, ProcessApplicInterface::multiple\_ParamsFiles, ProcessApplicInterface::FilterName, Interface::outputLevel, ProcessApplicInterface::program\_Names, WorkdirHelper::rename(), ProcessApplicInterface::specified\_ParamsFileName, ProcessApplicInterface::specified\_ResultsFileName, and ApplicationInterface::suppress\_Output.

Referenced by ProcessApplicInterface::read\_results\_files().

void synchronous\_local\_analyses (int start, int end, int step ) [inline], [protected]

execute analyses synchronously on the local processor

Execute analyses synchronously in succession on the local processor (start to end in step increments). Modeled after ApplicationInterface::synchronous\_local\_evaluations().

References ApplicationInterface::synchronous\_local\_analysis().

Referenced by ProcessHandleApplicInterface::create\_evaluation\_process().

void prepare\_process\_environment ( ) [protected]

set PATH, environment variables, and change directory prior to fork/system/spawn

Guidance: environment (PATH, current directory) should be set immediately before Dakota spawns a process and reset immediately afterwards (except fork which never returns)

References WorkdirHelper::change\_directory(), ProcessApplicInterface::cur\_Workdir, Interface::output\_Level, ProcessApplicInterface::params\_FileName, ProcessApplicInterface::results\_FileName, WorkdirHelper::set\_environment(), WorkdirHelper::set\_preferred\_path(), and ProcessApplicInterface::use\_Workdir.

Referenced by SpawnApplicInterface::create\_analysis\_process(), ForkApplicInterface::create\_analysis\_process(), SysCallApplicInterface::spawn\_analysis\_to\_shell(), SysCallApplicInterface::spawn\_evaluation\_to\_shell(), SysCallApplicInterface::spawn\_input\_filter\_to\_shell(), and SysCallApplicInterface::spawn\_output\_filter\_to\_shell().

void reset\_process\_environment ( ) [protected]

reset PATH and current directory after system/spawn (workdir case)

Undo anything done prior to spawn

References Interface::output\_Level, WorkdirHelper::reset(), WorkdirHelper::startup\_pwd(), and ProcessApplicInterface::use\_Workdir.

Referenced by SpawnApplicInterface::create\_analysis\_process(), ForkApplicInterface::create\_analysis\_process(), SysCallApplicInterface::spawn\_analysis\_to\_shell(), SysCallApplicInterface::spawn\_evaluation\_to\_shell(), SysCallApplicInterface::spawn\_input\_filter\_to\_shell(), and SysCallApplicInterface::spawn\_output\_filter\_to\_shell().

void read\_results\_file (Response & response, const bfs::path & path, const int id ) [private]

Open and read the results file at path, properly handling errors.

Helper for read\_results\_files that opens the results file at results\_path and reads it, handling various errors/exceptions.

References Dakota::abort\_handler(), Response::read(), and ProcessApplicInterface::results\_FileFormat.

Referenced by ProcessApplicInterface::read\_results\_files().

The documentation for this class was generated from the following files:

- ProcessApplicInterface.hpp
- ProcessApplicInterface.cpp
### 13.151 ProcessHandleApplicInterface Class Reference

Derived application interface class that spawns a simulation code using a separate process, receives a process identifier, and communicates with the spawned process through files.

Inheritance diagram for ProcessHandleApplicInterface:

```
    Interface
      |
      v
  ApplicationInterface
      |
      v
  ProcessApplicInterface
      |
      v
ProcessHandleApplicInterface
      |
      v
  ForkApplicInterface
      |
      v
  SpawnApplicInterface
```

#### Public Member Functions

- **ProcessHandleApplicInterface** (const ProblemDescDB &problem_db)
  
  *constructor*

- **~ProcessHandleApplicInterface** ()
  
  *destructor*

#### Protected Member Functions

- int **synchronous_local_analysis** (int analysis_id)
- void **init_communicators_checks** (int max_eval_concurrency)
- void **set_communicators_checks** (int max_eval_concurrency)
- void **map_bookkeeping** (pid_t pid, int fn_eval_id)
  
  *bookkeeping of process and evaluation ids for asynchronous maps*

- pid_t **create_evaluation_process** (bool block_flag)
- virtual pid_t **create_analysis_process** (bool block_flag, bool new_group)=0
  
  *spawn a child process for an analysis component within an evaluation*

- virtual size_t **wait_local_analyses** ()=0
  
  *wait for asynchronous analyses on the local processor, completing at least one job*

- virtual size_t **test_local_analyses_send** (int analysis_id)=0
  
  *test for asynchronous analysis completions on the local processor and return results for any completions by sending messages*

- virtual void **join_evaluation_process_group** (bool new_group)
  
  *create (if new_group) and join the process group for asynch evaluations*

- virtual void **join_analysis_process_group** (bool new_group)
  
  *create (if new_group) and join the process group for asynch analyses*

- virtual void **evaluation_process_group_id** (pid_t pgid)
set evalProcGroupId
• virtual pid_t evaluation_process_group_id () const
  return evalProcGroupId
• virtual void analysis_process_group_id (pid_t pgid)
  set analysisProcGroupId
• virtual pid_t analysis_process_group_id () const
  return analysisProcGroupId
• void process_local_evaluation (PRPQueue &prp_queue, const pid_t pid)
  Common processing code used by {wait,test} local evaluations.
• void check_wait (pid_t pid, int status)
  check the exit status of a forked process and abort if an error code was returned
• void asynchronous_local_analyses (int start, int end, int step)
  execute analyses asynchronously on the local processor
• void serve_analyses_asynch ()
  serve the analysis scheduler and execute analysis jobs asynchronously
• void ifilter_argument_list ()
  set argList for execution of the input filter
• void ofilter_argument_list ()
  set argList for execution of the output filter
• void driver_argument_list (int analysis_id)
  set argList for execution of the specified analysis driver
• void create_command_arguments (boost::shared_array<const char *> &av, StringArray &driver_and_args)
  parse argList into argument array av suitable for passing to execvp, appending parameters and results filenames if requested by commandLineArgs

Protected Attributes
• std::map< pid_t, int > evalProcessIdMap
  map of fork process id’s to function evaluation id’s for asynchronous evaluations
• std::map< pid_t, int > analysisProcessIdMap
  map of fork process id’s to analysis job id’s for asynchronous analyses
• std::vector< std::string > argList
  an array of strings for use with execvp(const char *, char const *). These are converted to an array of const char*’s in fork_program().

13.151.1 Detailed Description
Derived application interface class that spawns a simulation code using a separate process, receives a process identifier, and communicates with the spawned process through files.
  ProcessHandleApplicInterface is subclassed for fork/execvp/waitpid (Unix) and spawnvp (Windows).

13.151.2 Constructor & Destructor Documentation
ProcessHandleApplicInterface ( const ProblemDescDB & problem_db ) [inline]
constructor
argList sized 3 for [driver name, input file, output file]
13.151.3 Member Function Documentation

```cpp
int synchronous_local_analysis ( int analysis_id ) [inline], [protected], [virtual]
```

This code provides the derived function used by `ApplicationInterface::serve_analyses_synch()` as well as a convenience function for `ProcessHandleApplicInterface::synchronous_local_analyses()` below.

Reimplemented from `ApplicationInterface`.

References `ProcessHandleApplicInterface::create_analysis_process()`, and `ProcessHandleApplicInterface::driver_argument_list()`.

```cpp
void init_communicators_checks ( int max_eval_concurrency ) [inline], [protected], [virtual]
```

No derived interface plug-ins, so perform construct-time checks. However, process init issues as warnings since some contexts (e.g., `HierarchSurrModel`) initialize more configurations than will be used.

Reimplemented from `ApplicationInterface`.

References `ApplicationInterface::check_multiprocessor_analysis()`, and `ApplicationInterface::check_multiprocessor_asynchronous()`.

```cpp
void set_communicators_checks ( int max_eval_concurrency ) [inline], [protected], [virtual]
```

Process run-time issues as hard errors.

Reimplemented from `ApplicationInterface`.

References `Dakota::abort_handler()`, `ApplicationInterface::check_multiprocessor_analysis()`, and `ApplicationInterface::check_multiprocessor_asynchronous()`.

```cpp
pid_t create_evaluation_process ( bool block_flag ) [protected], [virtual]
```

Manage the input filter, 1 or more analysis programs, and the output filter in blocking or nonblocking mode as governed by `block_flag`. In the case of a single analysis and no filters, a single analysis is performed, while in other cases, an initial fork is reforked multiple times. Called from `derived_map()` with `block_flag == BLOCK` and from `derived_map_asynch()` with `block_flag == FALL_THROUGH`. Uses `create_analysis_process()` to spawn individual program components within the function evaluation.

Implements `ProcessApplicInterface`.

References `Dakota::abort_handler()`, `ProcessHandleApplicInterface::analysis_process_group_id()`, `ApplicationInterface::analysis_ServerId`, `ApplicationInterface::asyncLocalAnalysisConcurrency`, `ApplicationInterface::asyncLocalAnalysisFlag`, `ProcessHandleApplicInterface::asyncLocalAnalysisFlag`, `ParallelLibrary::barrier_e()`, `ProcessApplicInterface::commandLineArgs`, `ProcessHandleApplicInterface::create_analysis_process()`, `ProcessHandleApplicInterface::driver_argument_list()`, `ApplicationInterface::eaDedMasterFlag`, `ApplicationInterface::evalCommRank`, `ApplicationInterface::evalCommSize`, `ProcessHandleApplicInterface::evalProcessIdMap`, `ProcessHandleApplicInterface::evaluation_process_group_id()`, `ProcessHandleApplicInterface::iFilterName`, `ProcessHandleApplicInterface::join_evaluation_process_group()`, `ApplicationInterface::master_dynamic_schedule_analyses()`, `ProcessApplicInterface::multipleParamsFiles`, `ApplicationInterface::numAnalysisDrivers`, `ApplicationInterface::numAnalysisServers`, `ProcessHandleApplicInterface::oFilterName`, `ApplicationInterface::paramsFileName`, `ProcessApplicInterface::programNames`, `ProcessApplicInterface::resultsFileName`, `ProcessHandleApplicInterface::serve_analyses_synch()`, `ApplicationInterface::serve_analyses_synch()`, `ApplicationInterface::suppressOutput`, and `ProcessApplicInterface::synchronous_local_analyses()`.

```cpp
void check_wait ( pid_t pid, int status ) [protected]
```

check the exit status of a forked process and abort if an error code was returned
Check to see if the process terminated abnormally (WIFEXITED(status)()==0) or if either execvp or the application returned a status code of -1 (WIFEXITED(status)!==0 && (signed char)WEXITSTATUS(status)==-1). If one of these conditions is detected, output a failure message and abort. Note: the application code should not return a status code of -1 unless an immediate abort of dakota is wanted. If for instance, failure capturing is to be used, the application code should write the word "FAIL" to the appropriate results file and return a status code of 0 through exit().

References Dakota::abort_handler().

Referenced by ForkApplicInterface::create_analysis_process(), SpawnApplicInterface::test_local_analyses_send(), SpawnApplicInterface::test_local_evaluations(), ForkApplicInterface::wait(), SpawnApplicInterface::wait_local_analyses(), and SpawnApplicInterface::wait_local_evaluations().

```cpp
void asynchronous_local_analyses ( int start, int end, int step ) [protected]
```

execute analyses asynchronously on the local processor

- Schedule analyses asynchronously on the local processor using a dynamic scheduling approach (start to end in step increments). Concurrency is limited by asynchLocalAnalysisConcurrency. Modeled after ApplicationInterface::asynchronous_local_evaluations(). NOTE: This function should be elevated to ApplicationInterface if and when another derived interface class supports asynchronous local analyses.

References Dakota::abort_handler(), ProcessHandleApplicInterface::analysisProcessIdMap, ApplicationInterface::asynchLocalAnalysisConcurrency, ProcessHandleApplicInterface::create_analysis_process(), ProcessHandleApplicInterface::driver_argument_list(), ApplicationInterface::numAnalysisDrivers, and ProcessHandleApplicInterface::wait_local_analyses().

Referenced by ProcessHandleApplicInterface::create_evaluation_process().

```cpp
void serve_analyses_asynch ( ) [protected]
```

serve the analysis scheduler and execute analysis jobs asynchronously

- This code runs multiple asynch analyses on each server. It is modeled after ApplicationInterface::serve_evaluations_asynch(). NOTE: This fn should be elevated to ApplicationInterface if and when another derived interface class supports hybrid analysis parallelism.

References Dakota::abort_handler(), ProcessHandleApplicInterface::analysisProcessIdMap, ApplicationInterface::asynchLocalAnalysisConcurrency, ProcessHandleApplicInterface::create_analysis_process(), ProcessHandleApplicInterface::driver_argument_list(), ParallelLibrary::irecv_ea(), ApplicationInterface::numAnalysisDrivers, ApplicationInterface::parallelLib, ParallelLibrary::recv_ea(), ParallelLibrary::test(), and ProcessHandleApplicInterface::test_local_analyses_send().

Referenced by ProcessHandleApplicInterface::create_evaluation_process().

```cpp
void create_command_arguments ( boost::shared_array< const char * > & av, StringArray & driver_and_args ) [protected]
```

parse argList into argument array av suitable for passing to execvp, appending parameters and results filenames if requested by commandLineArgs

- This function will split the analysis command in argList[0] based on whitespace, but preserve spaces within quoted strings, such that quoted strings can be passed as single command arguments. NOTE: This function allocates memory in av that might be implicitly freed when the child exits (control never returns to caller). driver_and_args needs to be a return argument because av will contain pointers into its c_str()’s when done.

References ProcessHandleApplicInterface::argList, ProcessApplicInterface::commandLineArgs, and WorkdirHelper::tokenize_driver().

Referenced by SpawnApplicInterface::create_analysis_process(), and ForkApplicInterface::create_analysis_process().
13.152. PROGRAMOPTIONS CLASS REFERENCE

The documentation for this class was generated from the following files:

- ProcessHandleApplicInterface.hpp
- ProcessHandleApplicInterface.cpp

13.152 ProgramOptions Class Reference

ProgramOptions stores options whether from the CLH or from library user; initially valid only on worldRank = 0, but then broadcast in ParallelLibrary::push_output_tag()

Public Member Functions

- **ProgramOptions ()**
  
  default constructor (needed for default environment ctors and could be used by library clients to late update data)

- **ProgramOptions (int world_rank)**
  
  constructor that accepts world rank to help with I/O control; allows default constructed ProgramOptions to get rank in library mode

- **ProgramOptions (int argc, char **argv[], int world_rank)**
  
  standard constructor that uses a CommandLineHandler to parse user options

- const String & input_file () const

  Dakota input file base name (no tag)

- const String & input_string () const

  alternate Dakota input string literal

- bool echo_input () const

  is input echo specified?

- const String & parser_options () const

  (deprecated) NIDR parser options

- String output_file () const

  output (user-provided or default) file base name (no tag)

- const String & error_file () const

  error file base name (no tag)

- const String & exit_mode () const

  behavior of abort_handler (throw or exit)

- const String & read_restart_file () const

  restart file base name (no tag)

- size_t stop_restart_evals () const

  eval ID at which to stop reading restart

- String write_restart_file () const

  write restart (user-provided or default) file base name (no tag)

- bool help () const

  is help mode active?

- bool version () const

  is version mode active?

- bool check () const
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is check mode active?
• bool pre_run () const
  is pre-run mode active?
• bool run () const
  is run mode active?
• bool post_run () const
  is post-run mode active?
• bool user_modes () const
  are any non-default, user-specified run modes active?
• const String & pre_run_input () const
  filename for pre-run input
• const String & pre_run_output () const
  filename for pre-run output
• const String & run_input () const
  filename for run input
• const String & run_output () const
  filename for run output
• const String & post_run_input () const
  filename for post-run input
• const String & post_run_output () const
  filename for post-run output
• unsigned int pre_run_output_format () const
  tabular format for pre-run output
• unsigned int post_run_input_format () const
  tabular format for post-run input
• bool proceed_toInstantiate () const
  whether steps beyond help/version are requested (instantiation required)
• bool proceed_to_run () const
  Whether steps beyond check are requested.
• bool user_stdout_redirect () const
  whether the user/client code requested a redirect of stdout
• bool user_stderr_redirect () const
  whether the user/client code requested a redirect of stderr
• void world_rank (int world_rank)
  set the world rank to govern early conditional output
• void input_file (const String &in_file)
  set Dakota input file base name (no tag)
• void input_string (const String &in_string)
  set alternate Dakota input string literal
• void echo_input (bool echo_flag)
  set whether to echo input to output
• void exit_mode (const String &mode)
  set behavior for abort_handler
void output_file (const String &out_file)
    set base file name for Dakota output

void error_file (const String &err_file)
    set base file name for Dakota errors

void read_restart_file (const String &read_rst)
    set base file name for restart file from which to read

void stop_restart_evals (size_t stop_rst)
    set eval ID at which to stop reading restart

void write_restart_file (const String &write_rst)
    set base file name for restart file to write

void help (bool help_flag)
    set true to print help information and exit

void version (bool version_flag)
    set true to print version information and exit

void check (bool check_flag)
    set true to check input and instantiate objects, then exit

void pre_run (bool pre_run_flag)
    set to enable/disable pre-run phase

void run (bool run_flag)
    set to enable/disable run phase

void post_run (bool post_run_flag)
    set to enable/disable post-run phase

void pre_run_input (const String &pre_run_in)
    Specify the pre-run phase input filename.

void pre_run_output (const String &pre_run_out)
    Specify the pre-run phase output filename.

void run_input (const String &run_in)
    Specify the run phase input filename.

void run_output (const String &run_out)
    Specify the run phase output filename.

void post_run_input (const String &post_run_in)
    Specify the post-run phase input filename.

void post_run_output (const String &post_run_out)
    Specify the post-run phase output filename.

void parse (const ProblemDescDB &problem_db)
    Extract environment options from ProblemDescDB.

void read (MPIUnpackBuffer &s)
    helper function for reading some class data from MPI buffer

void write (MPIPackBuffer &s) const
    helper function for writing some class data to MPI buffer
Private Member Functions

- void parse_environment_options ()
  any environment variables affecting global behavior get read here
- void manage_run_modes (const CommandLineHandler &clh)
  retrieve run mode options from the CLH
- void split_filenames (const char *filenames, std::string &input_filename, std::string &output_filename)
  manage pre/run/post filenames
- void validate ()
  verify consistency of user settings (helpful for library mode especially)
- void validate_run_modes ()
  validate user run modes and set userModesFlag
- void set_option (const ProblemDescDB &problem_db, const String &db_name, String &data_member)
  retrieve environment.<db_name> from the problem db and update data_member, warning if needed

Private Attributes

- int worldRank
  cache the world rank to help with conditional output
- String inputFile
  Dakota input file name, e.g., “dakota.in”.
- String inputString
  alternate input means for library clients: input string (mutually exclusive with input file)
- bool echoInput
  whether to echo client’s input file at parse
- String parserOptions
  Deprecated option for NIDR parser options.
- String exitMode
  Abort or throw on error.
- String outputFile
  Dakota output base file name, e.g., “dakota.out”.
- String errorFile
  Dakota error base file name, e.g., “dakota.err”.
- String readRestartFile
  e.g., “dakota.old.rst”
- size_t stopRestartEvals
  eval number at which to stop restart read
- String writeRestartFile
  e.g., “dakota.new.rst”
- bool helpFlag
  whether to print help message and exit
- bool versionFlag
  whether to print version message and exit
- bool checkFlag
flags invocation with command line option -check

- bool preRunFlag

flags invocation with command line option -pre_run

- bool runFlag

flags invocation with command line option -run

- bool postRunFlag

flags invocation with command line option -post_run

- bool userModesFlag

whether any user run modes are active

- String preRunInput

  filename for pre_run input

- String preRunOutput

  filename for pre_run output

- String runInput

  filename for run input

- String runOutput

  filename for run output

- String postRunInput

  filename for post_run input

- String postRunOutput

  filename for post_run output

- unsigned short preRunOutputFormat

  tabular format for pre_run output

- unsigned short postRunInputFormat

  tabular format for post_run input

13.152.1 Detailed Description

ProgramOptions stores options whether from the CLH or from library user; initially valid only on worldRank = 0, but then broadcast in ParallelLibrary::push_output_tag()

13.152.2 Member Function Documentation

void split_filenames ( const char *filenames, std::string &input_filename, std::string &output_filename )

[private]

manage pre/run/post filenames

  Tokenize colon-delimited input and output filenames, returns unchanged strings if tokens not found.

  Referenced by ProgramOptions::manage_run_modes().

  The documentation for this class was generated from the following files:

- ProgramOptions.hpp
- ProgramOptions.cpp
13.153 PStudyDACE Class Reference

Base class for managing common aspects of parameter studies and design of experiments methods.

Inheritance diagram for PStudyDACE:

```
         Iterator
         |       
         v       
       Analyzer
          |       
PStudyDACE
          |       
         v       
DDACEDesignCompExp FSUDesignCompExp ParamStudy PSUADEDesignCompExp
```

Public Member Functions

- **bool resize ()**
  
  *reinitializes iterator based on new variable size*

Protected Member Functions

- **PStudyDACE (ProblemDescDB &problem db, Model &model)**
  
  *constructor*

- **PStudyDACE (unsigned short method name, Model &model)**
  
  *alternate constructor for instantiations "on the fly"*

- **~PStudyDACE ()**
  
  *destructor*

- **void print_results (std::ostream &s)**
  
  *print the final iterator results*

- **void volumetric_quality (int ndim, int num_samples, double *sample_points)**
  
  *Calculation of volumetric quality measures.*

Protected Attributes

- **SensAnalysisGlobal pStudyDACESensGlobal**
  
  *initialize statistical post processing*

- **bool volQualityFlag**
  
  *flag which specifies evaluation of volumetric quality measures*

- **bool varBasedDecompFlag**
  
  *flag which specifies calculating variance based decomposition sensitivity analysis metrics*
Private Attributes

- double chiMeas
  quality measure
- double dMeas
  quality measure
- double hMeas
  quality measure
- double tauMeas
  quality measure

Additional Inherited Members

13.153.1 Detailed Description

Base class for managing common aspects of parameter studies and design of experiments methods.

The PStudyDACE base class manages common data and functions, such as those involving the best solutions located during the parameter set evaluations or the printing of final results.

13.153.2 Member Function Documentation

void print_results ( std::ostream & s ) [protected], [virtual]
print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References PStudyDACE::chiMeas, Analyzer::compactMode, Model::continuous_variable_labels(), SensAnalysisGlobal::correlations_computed(), Model::discrete_int_variable_labels(), Model::discrete_real_variable_labels(), Model::discrete_string_variable_labels(), PStudyDACE::dMeas, PStudyDACE::hMeas, Iterator::iteratedModel, Analyzer::numLSqTerms, Analyzer::numObjFns, SensAnalysisGlobal::print_correlations(), Analyzer::print_results(), Analyzer::print_sobol_indices(), PStudyDACE::pStudyDACEsensGlobal, Model::response_labels(), PStudyDACE::tauMeas, PStudyDACE::varBasedDecompFlag, and PStudyDACE::volQualityFlag.

void volumetric_quality ( int ndim, int num_samples, double * sample_points ) [protected]
Calculation of volumetric quality measures.

Calculation of volumetric quality measures developed by FSU.

References PStudyDACE::chiMeas, PStudyDACE::dMeas, PStudyDACE::hMeas, and PStudyDACE::tauMeas.

Referenced by FSUDesignCompExp::get_parameter_sets(), and DDACEDesignCompExp::get_parameter_sets().
The documentation for this class was generated from the following files:

- DakotaPStudyDACE.hpp
- DakotaPStudyDACE.cpp
PSUADEDesignCompExp Class Reference

Wrapper class for the PSUADE library.

Inheritance diagram for PSUADEDesignCompExp:

```
  Iterator
   |
   Analyzer
   |
   PStudyDACE
   |
PSUADEDesignCompExp
```

Public Member Functions

- **PSUADEDesignCompExp** (ProblemDescDB &problem_db, Model &model)
  
  primary constructor for building a standard DACE iterator
- **~PSUADEDesignCompExp** ()
  
  destructor
- **bool resize ()**
  
  reinitializes iterator based on new variable size

Protected Member Functions

- **void pre_run ()**
  
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- **void post_input ()**
  
  read tabular data for post-run mode
- **void core_run ()**
  
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- **void post_run (std::ostream &s)**
  
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
- **int num_samples () const**
- **void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)**
  
  reset sampling iterator to use at least min_samples
- **unsigned short sampling_scheme () const**
  
  return sampling name
- **void vary_pattern (bool pattern_flag)**
  
  sets varyPattern in derived classes that support it
- **void get_parameter_sets (Model &model)**
  
  Generate one block of numSamples samples (ndim * num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
Private Member Functions

- void enforce_input_rules ()
  enforce sanity checks/modifications for the user input specification

Private Attributes

- int samplesSpec
  initial specification of number of samples
- int numSamples
  current number of samples to be evaluated
- const UShortArray & varPartitionsSpec
  number of partitions in each variable direction
- int numPartitions
  number of partitions to pass to PSUADE (levels = partitions + 1)
- bool allDataFlag
  flag which triggers the update of allVars/allResponses for use by Iterator::all_variables() and Iterator::all_responses()
- size_t numDACERuns
  counter for number of executions for this object
- bool varyPattern
  flag for generating a sequence of seed values within multiple get_parameter_sets() calls so that the sample sets are not repeated, but are still repeatable
- const int seedSpec
  the user seed specification for the random number generator (allows repeatable results)
- int randomSeed
  current seed for the random number generator

Additional Inherited Members

13.154.1 Detailed Description

Wrapper class for the PSUADE library.

The PSUADEDesignCompExp class provides a wrapper for PSUADE, a C++ design of experiments library from Lawrence Livermore National Laboratory. Currently this class only includes the PSUADE Morris One-at-a-time (MOAT) method to uniformly sample the parameter space spanned by the active bounds of the current Model. It returns all generated samples and their corresponding responses as well as the best sample found.

13.154.2 Constructor & Destructor Documentation

PSUADEDesignCompExp ( ProblemDescDB & problem_db, Model & model )

primary constructor for building a standard DACE iterator

This constructor is called for a standard iterator built with data from probDescDB.

References Dakota::abort_handler(), Iterator::maxEvalConcurrency, Iterator::method_string(), Iterator::method_Name, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, and PSUADEDesignCompExp::numSamples.
13.154.3 Member Function Documentation

void pre_run() [protected], [virtual]
pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s pre_run(), if implemented, typically before performing its own implementation steps.
Reimplemented from Analyzer.
References PSUADEDesignCompExp::enforce_input_rules(), PSUADEDesignCompExp::get_parameter_sets(), Iterator::iteratedModel, and Analyzer::pre_run().

void core_run() [protected], [virtual]
core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.
Reimplemented from Iterator.
References Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, Analyzer::numLSqTerms, and Analyzer::numObjFns.

void post_run( std::ostream &s ) [protected], [virtual]
post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s post_run(), typically after performing its own implementation steps.
Reimplemented from Analyzer.
References Dakota::abort_handler(), Analyzer::allResponses, Analyzer::allSamples, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), PSUADEDesignCompExp::enforce_input_rules(), Iterator::iteratedModel, Analyzer::numContinuousVars, Analyzer::numFunctions, PSUADEDesignCompExp::numSamples, and Analyzer::post_run().

int num_samples() const [inline], [protected], [virtual]
Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.
Reimplemented from Analyzer.
References PSUADEDesignCompExp::numSamples.

void enforce_input_rules() [private]
enforce sanity checks/modifications for the user input specification
Users may input a variety of quantities, but this function must enforce any restrictions imposed by the sampling algorithms.
References Analyzer::numContinuousVars, PSUADEDesignCompExp::numPartitions, PSUADEDesignCompExp::numSamples, and PSUADEDesignCompExp::varPartitionsSpec.
Referenced by PSUADEDesignCompExp::post_input(), PSUADEDesignCompExp::post_run(), and PSUADEDesignCompExp::pre_run().
The documentation for this class was generated from the following files:
13.155 PYTHONINTERFACE CLASS REFERENCE

- PSUADEDesignCompExp.hpp
- PSUADEDesignCompExp.cpp

13.155 PythonInterface Class Reference

Inheritance diagram for PythonInterface:

```
  Interface
  ApplicationInterface
  DirectApplicInterface
  PythonInterface
```

Public Member Functions

- **PythonInterface** (const ProblemDescDB &problem_db)
  
  constructor

- ∼**PythonInterface** ()
  
  destructor

Protected Member Functions

- virtual int **derived_map_ac** (const String &ac_name)
  
  execute an analysis code portion of a direct evaluation invocation

- int **python_run** (const String &ac_name)
  
  direct interface to Python via API, BMA 07/02/07

- template<class ArrayT, class Size>
  bool **python_convert_int** (const ArrayT &src, Size size, PyObject **dst)
  
  convert arrays of integer types to Python list or numpy array

- bool **python_convert** (const RealVector &src, PyObject **dst)
  
  convert RealVector to Python list or numpy array

- bool **python_convert** (const RealVector &c_src, const IntVector &di_src, const RealVector &dr_src, PyObject **dst)
  
  convert RealVector + IntVector + RealVector to Python mixed list or numpy double array

- template<class StringArrayT>
  bool **python_convert_strlist** (const StringArrayT &src, PyObject **dst)
  
  convert labels

- bool **python_convert** (const StringMultiArray &c_src, const StringMultiArray &di_src, const StringMultiArray &dr_src, PyObject **dst)
  
  convert all labels to single list

- bool **python_convert** (PyObject *pyv, RealVector &rv, const int &dim)
convert python [list of int or float] or [numpy array of double] to RealVector (for fns)

- bool python_convert (PyObject *pyv, double *rv, const int &dim)

convert python [list of int or float] or [numpy array of double] to double[], for use as helper in converting gradients

- bool python_convert (PyObject *pyv, RealMatrix &rm)

convert python [list of lists of int or float] or [numpy array of dbl] to RealMatrix (for gradients)

- bool python_convert (PyObject *pym, RealSymMatrix &rm)

convert python [list of lists of int or float] or [numpy array of dbl] to RealMatrix (used as helper in Hessian conversion)

- bool python_convert (PyObject *pyma, RealSymMatrixArray &rma)

convert python [list of lists of lists of int or float] or [numpy array of double] to RealSymMatrixArray (for Hessians)

Protected Attributes

- bool userNumpyFlag
  whether the user requested numpy data structures in the input file

- bool ownPython
  true if this class created the interpreter instance

13.155.1 Detailed Description

Specialization of DirectApplicInterface to link to Python analysis drivers. Includes convenience functions to map data to/from Python

13.155.2 Member Function Documentation

int derived_map_ac ( const String & ac_name ) [protected], [virtual]

execute an analysis code portion of a direct evaluation invocation

  Python specialization of derived analysis components.
  Reimplemented from DirectApplicInterface.
  References ApplicationInterface::analysisServerId, and PythonInterface::python_run().

bool python_convert_int ( const ArrayT & src, Size sz, PyObject ** dst ) [protected]

convert arrays of integer types to Python list or numpy array

  convert all integer array types including IntVector, ShortArray, and SizetArray to Python list of ints or numpy array of ints

  References PythonInterface::userNumpyFlag.
  Referenced by PythonInterface::python_run().

  The documentation for this class was generated from the following files:

  - PythonInterface.hpp
  - PythonInterface.cpp

13.156 QuesoJointPdf< V, M > Class Template Reference

Dakota specialization of QUESO generic joint PDF.

Inherits BaseJointPdf< V, M >. 
Public Member Functions

- QuesoJointPdf (const char *prefix, const QUESO::VectorSet< V, M > &domainSet, NonDQUESOBayesCalibration *nond_queso_ptr)
  Default constructor.
- virtual ~QuesoJointPdf ()
  Destructor.
- double actualValue (const V &domainVector, const V *domainDirection, V *gradVector, M *hessianMatrix, V *hessianEffect) const
  Actual value of the PDF (scalar function).
- double lnValue (const V &domainVector, const V *domainDirection, V *gradVector, M *hessianMatrix, V *hessianEffect) const
  Logarithm of the value of the function.
- double computeLogOfNormalizationFactor (unsigned int numSamples, bool m_logOfNormalizationFactor) const
  Computes the logarithm of the normalization factor.
- void distributionMean (V &meanVector) const
  Mean value of underlying random variable.
- void distributionVariance (M &covMatrix) const

Private Attributes

- NonDQUESOBayesCalibration * nonDQUESOInstance

13.156.1 Detailed Description

template<class V, class M>class Dakota::QuesoJointPdf< V, M >

Dakota specialization of QUESO generic joint PDF.

13.156.2 Constructor & Destructor Documentation

QuesoJointPdf ( const char * prefix, const QUESO::VectorSet< V, M > & domainSet, NonDQUESOBayesCalibration * nond_queso_ptr )

Default constructor.
Instantiates an object of the class, i.e. a scalar function, given a prefix and its domain.
The documentation for this class was generated from the following file:

- NonDQUESOBayesCalibration.cpp

13.157 QuesoVectorRV< V, M > Class Template Reference

Dakota specialization of QUESO vector-valued random variable.
Inherits BaseVectorRV< V, M >.
Public Member Functions

- **QuesoVectorRV** (const char *prefix, const QUESO::VectorSet<V, M> &imageSet, NonDQUESOBayesCalibration *nond_queso_ptr)
  Default constructor.
- **virtual ~QuesoVectorRV ()**
  Virtual destructor.
- **void print (std::ostream &os) const**
  *TODO:* Prints the vector RV (required pure virtual).

13.157.1 Detailed Description

template<class V, class M> class Dakota::QuesoVectorRV<V, M>

Dakota specialization of QUESO vector-valued random variable.

13.157.2 Constructor & Destructor Documentation

QuesoVectorRV ( const char *prefix, const QUESO::VectorSet<V, M> &imageSet, NonDQUESOBayesCalibration *nond_queso_ptr )

Default constructor.
Constructs a generic queso vector RV, given a prefix and the image set of the vector RV.
The documentation for this class was generated from the following file:

- NonDQUESOBayesCalibration.cpp

13.158 RandomFieldModel Class Reference

Random field model, capable of generating and then forward propagating.
Inheritance diagram for RandomFieldModel:

```
Model
|
---
RecastModel
|
---
RandomFieldModel
```

Public Member Functions

- **RandomFieldModel** (ProblemDescDB &problem_db)
  Problem database constructor.
- **~RandomFieldModel ()**
  Destructor
- **bool initialize_mapping** (ParLevLIter pl_iter)
  for KL models, the model is augmented with the random coeffs of the KL
• bool finalize_mapping ()
  finalize model mapping, returns true if the variables size has changed

• bool mapping_initialized () const
  return true if mapping has been fully initialized, false otherwise.

• bool resize_pending () const
  return true if a potential resize is still pending, such that sizing-based initialization should be deferred

Protected Member Functions

• Model get_sub_model (ProblemDescDB &problem_db)
  retrieve the sub-Model from the DB to pass up the constructor chain

• void init_dace_iterator (ProblemDescDB &problem_db)
  initialize the RF-generating sampler

• void validate_inputs ()
  validate the build controls and set defaults

• void get_field_data ()
  Source data generation: get the field data either from file or simulation by running the DACE Iterator. Populates rfBuildData.

• void identify_field_model ()
  Generate field representation: generate a KL or PCA/GP.

• void rf_suite_identify_field_model ()
  Generate field representation: utilize RF Suite.

• void initialize_recast ()
  Initialize the base class RecastModel with reduced space variable sizes.

• SizetArray variables_resize ()
  Create a variables components totals array with the reduced space size for continuous variables.

• void initialize_rf_coeffs ()
  For KL models, augment the subModel’s uncertain variables with additional N(0,1) variables; set up AleatoryDist-Params for the N(0,1)’s.

• void derived_evaluate (const ActiveSet &set)
  generate a random field realization, then evaluate the submodel

• void derived_evaluate_nowait (const ActiveSet &set)
  generate a random field realization, then evaluate the submodel (asynch)

• void generate_kl_realization ()
  generate a KL realization and write to file

• void generate_pca_gp_realization ()
  generate a PCA/GP realization and write to file

• void write_field (const RealVector &field_prediction)
  write a field realization to console and file
Static Protected Member Functions

- static void vars_mapping (const Variables &recast_xi_vars, Variables &sub_model_x_vars)
  map the active continuous recast variables to the active submodel variables (linear transformation)
- static void set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)
  map the inbound ActiveSet to the sub-model (map derivative variables)

Protected Attributes

- size_t numFunctions
- String rfDataFilename
  name of the data file with RF build data
- size_t numObservations
  rows of data matrix
- IntVector fieldLengths
  column partitions of data matrix
- RealMatrix rfBuildData
  data matrix with realizations of the random field to approximate
- RealMatrix rfBuildVars
  matrix of samples used to build the RF data
- Iterator daceIterator
  String dataDirectoryBasename;
- unsigned short expansionForm
  unsigned short analyticCovForm;
- unsigned short covarianceForm
  form of the analytic covariance function
- int requestedReducedRank
  current approximation of system rank
- Real percentVariance
  fraction of energy to capture
- int actualReducedRank
  command to run RF Suite
- ReducedBasis rfBasis
  reduced basis representation (for KL or PCA case)
- int fieldRealizationId
  counter for RF Suite
- std::vector< Approximation > gpApproximations
  approximate models used to map the uncertain vars through the PCA approx
- bool mappingInitialized
  the index of the active metaiterator-iterator parallelism level (corresponding to ParallelConfiguration::miPLIters)
  used at runtime
Static Protected Attributes

- static RandomFieldModel * rfmInstance
  
  static pointer to this class for use in static callbacks

Additional Inherited Members

13.158.1 Detailed Description

Random field model, capable of generating and then forward propagating.

Specialization of a RecastModel that optionally identifies an approximate random field model during build phase and creates a RecastModel capable of performing forward UQ including the field and auxiliiary uncertain variables reduced space. This RandomFieldModel wraps the random field propagation model (not the RF-generating model)

13.158.2 Member Function Documentation

**bool initialize_mapping ( ParLevLIter pl_iter ) [virtual]**

for KL models, the model is augmented with the random coeffs of the KL

May eventually take on init_comms and related operations. Also may want ide of build/update like DataFit-SurrModel, eventually.

Reimplemented from Model.

References RandomFieldModel::covarianceForm, Model::estimate_message_lengths(), RandomFieldModel::expansionForm, RandomFieldModel::fieldRealizationId, RandomFieldModel::get_field_data(), RandomFieldModel::identify_field_model(), RecastModel::initialize_mapping(), RandomFieldModel::initialize_recast(), RandomFieldModel::initialize_rf_coeffs(), RandomFieldModel::mappingInitialized, and RandomFieldModel::rf_suite_identify_field_model().

**void get_field_data ( ) [protected]**

Source data generation: get the field data either from file or simulation by running the DACE Iterator. Populates rfBuildData.

Populate rfBuildData

References Iterator::all_responses(), Iterator::all_samples(), Dakota::copy_data(), Model::cv(), RandomFieldModel::daceIterator, RandomFieldModel::expansionForm, Iterator::is_null(), Iterator::num_samples(), RandomFieldModel::rfBuildData, RandomFieldModel::rfBuildVars, Iterator::run(), and RecastModel::subModel.

Referenced by RandomFieldModel::initialize_mapping().

**void rf_suite_identify_field_model ( ) [protected]**

Generate field representation: utilize RF Suite.

Alternative to below function when using RFSuite.

References RandomFieldModel::actualReducedRank, and RandomFieldModel::requestedReducedRank.

Referenced by RandomFieldModel::initialize_mapping().

**void initialize_recast ( ) [protected]**

Initialize the base class RecastModel with reduced space variable sizes.

Initialize the recast model to augment the uncertain variables with actualReducedRank additional N(0,1) variables, with no response function mapping (for now).
References RandomFieldModel::actualReducedRank, Model::aleatory_distribution_parameters(), Model::current_response(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), Response::function_gradients(), Response::function_hessians(), RecastModel::init_maps(), RecastModel::init_sizes(), Model::num_functions(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), RandomFieldModel::rfmInstance, RandomFieldModel::set_mapping(), RecastModel::subModel, RandomFieldModel::variables_resize(), and RandomFieldModel::vars_mapping().

Referenced by RandomFieldModel::initialize_mapping().

SizeTArray variables_resize () [protected]
Create a variables components totals array with the reduced space size for continuous variables.
Create a variables components totals array with the reduced space size for continuous variables TODO: augment normal uncVars for KL case.
References RandomFieldModel::actualReducedRank, SharedVariablesData::components_totals(), Model::current_variables(), RandomFieldModel::expansionForm, Variables::shared_data(), RecastModel::subModel, and Dakota::svd().
Referenced by RandomFieldModel::initialize_recast().

void initialize_rf_coeffs () [protected]
For KL models, augment the subModel’s uncertain variables with additional N(0,1) variables; set up AleatoryDistParams for the N(0,1)’s.
Initialize the aleatory dist params for the KL coeffs
References RandomFieldModel::actualReducedRank, Model::aleatory_distribution_parameters(), Variables::continuous_variable_label(), Model::continuous_variable_labels(), Model::currentVariables, RandomFieldModel::expansionForm, RandomFieldModel::rfmInstance, and RecastModel::subModel.
Referenced by RandomFieldModel::initialize_mapping().

void vars_mapping ( const Variables & recast_xi_vars, Variables & sub_model_x_vars ) [static], [protected]
map the active continuous recast variables to the active submodel variables (linear transformation)
map the active continuous recast variables to the active submodel variables
References Variables::active_variables(), RandomFieldModel::actualReducedRank, Model::aleatory_distribution_parameters(), Variables::continuous_variables(), Model::cv(), Variables::discrete_int_variables(), Model::discrete_int_variables(), Variables::discrete_real_variables(), Model::discrete_real_variables(), Variables::discrete_string_variables(), Model::discrete_string_variables(), RandomFieldModel::expansionForm, RandomFieldModel::rfmInstance, and RecastModel::subModel.
Referenced by RandomFieldModel::initialize_recast().

13.158.3 Member Data Documentation

Iterator daceIterator [protected]
String dataDirectoryBasename;
DACE Iterator to evaluate the RF generating model
Referenced by RandomFieldModel::get_field_data(), RandomFieldModel::init_dace_iterator(), and RandomFieldModel::validate_inputs().
**unsigned short expansionForm**  [protected]

unsigned short analyticCovForm;
    form of the RF representation (KL, PCA, ICA)
    Referenced by RandomFieldModel::derived_evaluate(), RandomFieldModel::derived_evaluate_nowait(), RandomFieldModel::get_field_data(), RandomFieldModel::identify_field_model(), RandomFieldModel::initialize_mapping(), RandomFieldModel::initialize_rf_coeffs(), RandomFieldModel::resize_pending(), RandomFieldModel::variables_resize(), and RandomFieldModel::vars_mapping().

**int actualReducedRank**  [protected]

calculate command to run RF Suite
    number of bases retained in decomposition
    Referenced by RandomFieldModel::generate_kl_realization(), RandomFieldModel::generate_pca_gp_realization(), RandomFieldModel::identify_field_model(), RandomFieldModel::initialize_recast(), RandomFieldModel::initialize_rf_coeffs(), RandomFieldModel::rf_suite_identify_field_model(), RandomFieldModel::variables_resize(), and RandomFieldModel::vars_mapping().

**RandomFieldModel * rfInst**  [static], [protected]

static pointer to this class for use in static callbacks
    initialization of static needed by RecastModel
    Referenced by RandomFieldModel::initialize_recast(), RandomFieldModel::RandomFieldModel(), and RandomFieldModel::vars_mapping().

**bool mappingInitialized**  [protected]

the index of the active metaiterator-iterator parallelism level (corresponding to ParallelConfiguration::miPLIers) used at runtime
    track use of initialize_mapping() and finalize_mapping()
    Referenced by RandomFieldModel::finalze_mapping(), RandomFieldModel::initialize_mapping(), RandomFieldModel::mapping_initialized(), and RandomFieldModel::resize_pending().

The documentation for this class was generated from the following files:

- RandomFieldModel.hpp
- RandomFieldModel.cpp

# 13.159 RecastModel Class Reference

Derived model class which provides a thin wrapper around a sub-model in order to recast the form of its inputs and/or outputs.

Inheritance diagram for RecastModel:
Public Member Functions

  
  Standard (full) constructor; assumes provided sizes and map functions are final and constructs all member data

- **RecastModel** (const Model &sub_model, const SizetArray &vars_comps_totals, const BitArray &all_relax_di, const BitArray &all_relax_dr, size_t num_recast_primary_fns, size_t num_recast_secondary_fns, size_t recast_secondary_offset, short recastResp_order)
  
  Alternate constructor; uses provided sizes to construct Variables, Response and Constraints so Model can be passed to an Iterator; requires subsequent initMaps() call.

- **RecastModel** (ProblemDescDB &problem_db, const Model &sub_model)
  
  Problem DB-based ctor, e.g., for use in subspace model; assumes mappings to be initialized later; only initializes based on sub-model.

- **RecastModel** (const Model &sub_model)

  Lightest constructor used when transform sizes aren’t known at construct time; doesn’t initialize variables and responses, so this Model can’t be used to construct an Iterator; requires subsequent initSizes() and initMaps() calls.

- **~RecastModel** ()

  Destructor

- void **initSizes** (const SizetArray &vars_comps_totals, const BitArray &all_relax_di, const BitArray &all_relax_dr, size_t num_recast_primary_fns, size_t num_recast_secondary_fns, size_t recast_secondary_offset, short recastResp_order)

  Update recast sizes and size Variables and Response members after alternate construction


  Initialize recast indices and map callbacks after alternate construction

- void **inverseMappings** (void(*inv_vars_map)(const Variables &sub_model_vars, Variables &recast_vars), void(*inv_set_map)(const Variables &sub_model_vars, const ActiveSet &sub_model_set, ActiveSet &recast_set), void(*inv_priResp_map)(const Variables &recast_vars, const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp), void(*inv_secResp_map)(const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp))

  Provide optional inverse mappings

- void **transformVariables** (const Variables &recast_vars, Variables &sub_model_vars)

  Perform transformation of Variables (recast \(\rightarrow\) sub-model)

- void **transformSet** (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)
• void transform_response (const Variables &recast_vars, const Variables &sub_model_vars, const Response &sub_model Resp, Response &recastResp)
  perform transformation of Response (sub-model -> recast)
• void transform_response_map (const IntResponseMap &oldResp_map, IntResponseMap &newResp_map)
  invoke transform_response() on each response within oldResp_map to create newResp_map
• void inverse_transform_variables (const Variables &sub_model_vars, Variables &recast_vars)
  perform inverse transformation of Variables (sub-model -> recast)
• void inverse_transform_set (const Variables &sub_model_vars, const ActiveSet &sub_model_set, ActiveSet &recast_set)
  into sub_model_set for use with subModel.
• void inverse_transform_response (const Variables &sub_model_vars, const Variables &recast_vars, const Response &recastResp, Response &sub_modelResp)
  perform inverse transformation of Response (recast -> sub-model)
• void submodel_supports_derivative_estimation (bool sed_flag)
  override the submodel’s derivative estimation behavior

Protected Member Functions

• bool initialize_mapping (ParLevLIter pL_iter)
  initialize model mapping, returns true if the variables size has changed
• bool finalize_mapping ()
  finalize model mapping, returns true if the variables size has changed
• void derived_evaluate (const ActiveSet &set)
  portion of evaluate() specific to RecastModel (forward to subModel.evaluate())
• void derived_evaluate_nowait (const ActiveSet &set)
  portion of evaluate_nowait() specific to RecastModel (forward to subModel.evaluate_nowait())
• const IntResponseMap & derived_synchronize ()
  portion of synchronize() specific to RecastModel (forward to subModel.synchronize())
• const IntResponseMap & derived_synchronize_nowait ()
  portion of synchronize_nowait() specific to RecastModel (forward to subModel.synchronize_nowait())
• Iterator & subordinate_iterator ()
  return sub-iterator, if present, within subModel
• Model & subordinate_model ()
  return subModel
• Model & surrogate_model ()
  return surrogate model, if present, within subModel
• Model & truth_model ()
  return truth model, if present, within subModel
• void derived_subordinate_models (ModelList &ml, bool recurse_flag)
  add subModel to list and recurse into subModel
• void update_from_subordinate_model (size_t depth=std::numeric_limits< size_t >::max())
  pass request to subModel if recursing and then update from it
• Interface & derived_interface ()
return subModel interface

- `size_t solution_levels() const`
  return size of subModel::solnControlCostMap

- `void solution_level_index(size_t lev_index)`
  activate entry in subModel::solnControlCostMap

- `RealVector solution_level_cost() const`
  return cost estimates from subModel::solnControlCostMap

- `void primary_response_fn_weights(const RealVector &wts, bool recurse_flag=true)`
  set the relative weightings for multiple objective functions or least squares terms and optionally recurses into sub-Model

- `void surrogate_function_indices(const IntSet &surr_fn_indices)`
  update the subModel’s surrogate response function indices (DataFitSurrModel::surrogateFnIndices)

- `void surrogate_response_mode(short mode)`
  update the subModel’s surrogate response mode (SurrogateModel::responseMode)

- `void build_approximation()`
  builds the subModel approximation

- `bool build_approximation(const Variables &vars, const IntResponsePair &response_pr)`
  builds the subModel approximation

- `void update_approximation(bool rebuild_flag)`
  replaces data in the subModel approximation

- `void update_approximation(const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)`
  replaces data in the subModel approximation

- `void update_approximation(const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)`
  replaces data in the subModel approximation

- `void append_approximation(bool rebuild_flag)`
  appends data to the subModel approximation

- `void append_approximation(const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)`
  appends data to the subModel approximation

- `void append_approximation(const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)`
  appends data to the subModel approximation

- `void pop_approximation(bool save_surr_data, bool rebuild_flag=false)`
  remove the previous data set addition to a surrogate (e.g., due to a previous append_approximation() call); flag manages storing of surrogate data for use in a subsequent push_approximation()

- `void push_approximation()`
  push a previous approximation data state; reverse of pop_approximation

- `bool push_available()`
  query for whether a trial increment is restorable within a surrogate

- `void finalize_approximation()`
  finalize an approximation by applying all previous trial increments

- `void store_approximation(size_t index=NPOS)`
  move the current approximation into storage for later combination; the index of the stored set can be passed to allow replacement instead of augmentation (default is push_back)
void restore_approximation (size_t index=NPOS)

return an approximation from storage; the index identifies a particular stored data set (default is pop_back from stored)

void remove_stored_approximation (size_t index=NPOS)

remove a stored approximation, due to redundancy with the current approximation, prior to combination (default for no index is pop_back)

void combine_approximation (short corr_type)

combine the current approximation with previously stored data sets

std::vector< Approximation > & approximations ()

retrieve the set of Approximations from the subModel

const RealVectorArray & approximation_coefficients (bool normalized=false)

retrieve the approximation coefficients from the subModel

void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)

set the approximation coefficients within the subModel

const RealVector & approximation_variances (const Variables &vars)

retrieve the approximation variances from the subModel

const Pecos::SurrogateData & approximation_data (size_t index)

retrieve the approximation data from the subModel

void component_parallel_mode (short mode)

RecastModel only supports parallelism in subModel, so this virtual function redefinition is simply a sanity check.

size_t mi_parallel_level_index () const

return subModel’s MI parallel level index

short local_eval_synchronization ()

return subModel local synchronization setting

int local_eval_concurrency ()

return subModel local evaluation concurrency

bool derived_master_overload () const

flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to subModel)

IntIntPair estimate_partition_bounds (int max_eval_concurrency)

estimate the minimum and maximum partition sizes that can be utilized by this Model

void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

set up RecastModel for parallel operations (request forwarded to subModel)

void derived_init_serial ()

set up RecastModel for serial operations (request forwarded to subModel).

void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

set active parallel configuration within subModel

void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

deallocate communicator partitions for the RecastModel (request forwarded to subModel)

void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

Service subModel job requests received from the master. Completes when a termination message is received from stop_servers().

void stop_servers ()

executed by the master to terminate subModel server operations when RecastModel iteration is complete.

void inactive_view (short view, bool recurse_flag=true)
update the Model's inactive view based on higher level (nested) context and optionally recurse into subModel

- **const String & interface_id () const**
  return the subModel interface identifier

- **bool evaluation_cache (bool recurse_flag=true) const**
  if recurse_flag, return the subModel evaluation cache usage

- **bool restart_file (bool recurse_flag=true) const**
  if recurse_flag, return the subModel restart file usage

- **int derived_evaluation_id () const**
  return the current evaluation id for the RecastModel

- **void set_evaluation_reference ()**
  set the evaluation counter reference points for the RecastModel (request forwarded to subModel)

- **void fine_grained_evaluation_counters ()**
  request fine-grained evaluation reporting within subModel

- **void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const**
  print the evaluation summary for the RecastModel (request forwarded to subModel)

- **void warm_start_flag (const bool flag)**
  set the warm start flag, including the orderedModels

- **void eval_tag_prefix (const String &eval_id_str)**
  set the hierarchical eval ID tag prefix

- **bool dbLookup (const Variables &search_vars, const ActiveSet &search_set, Response &found_resp)**
  RecastModel may need to map variables, asv before DB lookup, or responses after lookup.

- **bool init_variables (const SizetArray &vars_comps_totals, const BitArray &all_relax_di, const BitArray &all_relax_dr)**
  initialize currentVariables and related info from the passed size/type info

- **void init_response (size_t num_recast_primary_fns, size_t num_recast_secondary_fns, short recast_resp_order, bool reshape_vars)**
  initialize currentResponse from the passed size info

- **void reshape_response (size_t num_recast_primary_fns, size_t num_recast_secondary_fns)**
  Reshape the RecastModel Response, assuming no change in variables or derivative information.

- **void init_constraints (size_t num_recast_secondary_fns, size_t recast_secondary_offset, bool reshape_vars)**
  initialize userDefinedConstraints from the passed size info

### Protected Attributes

- **Model subModel**
  the sub-model underlying the transformations

- **int recastModelEvalCntr**
  local evaluation id counter used for id mapping

- **IntActiveSetMap recastSetMap**
  map of recast active set passed to derived_evaluate_nowait(). Needed for currentResponse update in synchronization routines.

- **IntVariablesMap recastVarsMap**
map of recast variables used by derived_evaluate_nowait(). Needed for primaryRespMapping() and secondaryRespMapping() in synchronization routines.

- **IntVariablesMap subModelVarsMap**
  map of subModel variables used by derived_evaluate_nowait(). Needed for primaryRespMapping() and secondaryRespMapping() in synchronization routines.

- **IntResponseMap recastResponseMap**
  map of recast responses used by RecastModel::derived_synchronize() and RecastModel::derived_synchronize_nowait()

- **IntIntMap recastIdMap**
  mapping from subModel evaluation ids to RecastModel evaluation ids

### Private Member Functions

- **void initialize_data_from_submodel ()**
  code shared among constructors to initialize base class data from submodel

- **void update_from_submodel ()**
  update current variables/labels/bounds/targets from subModel

### Private Attributes

- **Sizet2DArray varsMapIndices**
  For each subModel variable, identifies the indices of the recast variables used to define it (maps RecastModel variables to subModel variables; data is packed with only the variable indices employed rather than a sparsely filled \( N_{sm} \times N_r \) matrix).

- **bool nonlinearVarsMapping**
  boolean set to true if the variables mapping involves a nonlinear transformation. Used in transform_set() to manage the requirement for gradients within the Hessian transformations. This does not require a BoolDeque for each individual variable, since response gradients and Hessians are managed per function, not per variable.

- **bool respMapping**
  set to true if non-NULL primaryRespMapping or secondaryRespMapping are supplied

- **Sizet2DArray primaryRespMapIndices**
  For each recast primary function, identifies the indices of the subModel functions used to define it (maps subModel response to RecastModel Response).

- **Sizet2DArray secondaryRespMapIndices**
  For each recast secondary function, identifies the indices of the subModel functions used to define it (maps subModel response to RecastModel response).

- **BoolDequeArray nonlinearRespMapping**
  array of BoolDeques, one for each recast response function. Each BoolDeque defines which subModel response functions contribute to the recast function using a nonlinear mapping. Used in transform_set() to augment the subModel function value/gradient requirements.

- **void(* variablesMapping ) (const Variables &recast_vars, Variables &sub_model_vars)**
  holds pointer for variables mapping function passed in ctor/initialize

- **void(* setMapping ) (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)**
  holds pointer for set mapping function passed in ctor/initialize

- **void(* primaryRespMapping ) (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)**
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holds pointer for primary response mapping function passed in ctor/initialize


holds pointer for secondary response mapping function passed in ctor/initialize

- void(* invVarsMapping)(const Variables &sub_model_vars, Variables &recast_vars)

holds pointer for optional inverse variables mapping function passed in inverse_mappings()

- void(* invSetMapping)(const Variables &sub_model_vars, const ActiveSet &sub_model_set, ActiveSet &recast_set)

holds pointer for optional inverse set mapping function passed in inverse_mappings()

- void(* invPriRespMapping)(const Variables &recast_vars, const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp)

holds pointer for optional inverse primary response mapping function passed in inverse_mappings()

- void(* invSecRespMapping)(const Variables &recast_vars, const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp)

holds pointer for optional inverse secondary response mapping function passed in inverse_mappings()

Additional Inherited Members

13.159.1 Detailed Description

Derived model class which provides a thin wrapper around a sub-model in order to recast the form of its inputs and/or outputs.

The RecastModel class uses function pointers to allow recasting of the subModel input/output into new problem forms. For example, this is used to recast SBO approximate subproblems, multiobjective and least-squares reductions, and variable/response.

For now, making the assumption that variables mappings are ordered by submodel active continuous, discrete int, discrete string, discrete real variables, even though all current use cases are continuous only.

When not using the standard (full) constructor, client code must make sure to complete initialization before using the RecastModel’s mapping functions. Initialization steps:

1. sub model (all ctors do this)
2. init_sizes: once known, size Variables, Response, Constraints (full and intermediate ctor do this)
3. init_maps: set indices and callback pointers (only full ctor does this)

13.159.2 Constructor & Destructor Documentation

RecastModel ( const Model & sub_model, const Sizet2DArray & vars_map_indices, const SizetArray & vars_comps_totals, const BitArray & all_relax_di, const BitArray & all_relax_dr, bool nonlinear_vars_mapping, void(*)(const Variables &recast_vars, Variables &sub_model_vars) variables_map, void(*)(const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set) set_map, const Sizet2DArray & primary_resp_map_indices, const Sizet2DArray & secondary_resp_map_indices, size_t recast_secondary_offset, short recast_resp_order, const BoolDequeArray & nonlinearRespMapping, void(*)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response) primary_resp_map, void(*)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response) secondary_resp_map )

standard (full) constructor; assumes provided sizes and map functions are final and constructs all member data
13.159. RECASTMODEL CLASS REFERENCE

Default recast model constructor. Requires full definition of the transformation; if any mappings are NULL, they are assumed to remain so in later initialization or updates. Parameter vars\_comps\_totals indicates the number of each type of variable \(4\ \text{types} \times 3\ \text{domains}\) in the recast variable space. Note: recast\_secondary\_offset is the start index for equality constraints, typically num nonlinear ineq constraints.

References Dakota::abort\_handler(), Response::copy(), Variables::copy(), Model::current\_response(), Model::current\_variables(), Model::current\_Response, Model::current\_Variables, Variables::cv(), RecastModel::init\_constraints(), RecastModel::init\_response(), RecastModel::init\_variables(), RecastModel::initialize\_data\_from\_submodel(), Model::model\_Type, RecastModel::nonlinear\_Resp\_Mapping, Response::num\_functions(), Model::num\_Deriv\_Vars, Model::num\_Fns, RecastModel::primary\_Resp\_Map\_Indices, RecastModel::primary\_Resp\_Mapping, RecastModel::resp\_Mapping, RecastModel::secondary\_Resp\_Map\_Indices, RecastModel::secondary\_Resp\_Mapping, RecastModel::sub\_Model, Model::supports\_Estim\_Derivs, and RecastModel::variables\_Mapping.

**RecastModel**

\[
\text{RecastModel ( const Model & sub\_model, const Sizet\_Array & vars\_comps\_totals, const Bit\_Array & all\_relax\_di, const Bit\_Array & all\_relax\_dr, size\_t num\_recast\_primary\_fns, size\_t num\_recast\_secondary\_fns, size\_t recast\_secondary\_offset, short recast\_resp\_order )}
\]

alternate constructor; uses provided sizes to construct Variables, Response and Constraints so Model can be passed to an Iterator; requires subsequent init\_maps() call.

This alternate constructor defers initialization of the function pointers until a separate call to initialize(), and accepts the minimum information needed to construct current\_Variables, current\_Response, and user\_Defined\_Constraints. The resulting model is sufficiently complete for passing to an Iterator. Parameter vars\_comps\_totals indicates the number of each type of variable \(4\ \text{types} \times 3\ \text{domains}\) in the recast variable space. Note: recast\_secondary\_offset is the start index for equality constraints, typically num nonlinear ineq constraints.

References RecastModel::init\_sizes(), RecastModel::initialize\_data\_from\_submodel(), Model::model\_Type, and Model::supports\_Estim\_Derivs.

13.159.3 Member Function Documentation

**void init\_maps ( const Sizet\_2D\_Array & vars\_map\_indices, bool nonlinear\_vars\_mapping, void(*)\(\text{const Variables &recast\_vars, Variables &sub\_model\_vars}\) variables\_map, void(*)\(\text{const Variables &recast\_vars, const Active\_Set &recast\_set, Active\_Set &sub\_model\_set}\) set\_map, const Sizet\_2D\_Array & primary\_resp\_map\_indices, const Sizet\_2D\_Array & secondary\_resp\_map\_indices, const Bool\_Deque\_Array & nonlinear\_resp\_mapping, void(*)\(\text{const Variables &sub\_model\_vars, const Variables &recast\_vars, const Response &sub\_model\_response, Response &recast\_response}\) primary\_resp\_map, void(*)\(\text{const Variables &sub\_model\_vars, const Variables &recast\_vars, const Response &sub\_model\_response, Response &recast\_response}\) secondary\_resp\_map \)**

initialize recast indices and map callbacks after alternate construction

This function is used for late initialization of the recasting functions. It is used in concert with the alternate constructor.

References Dakota::abort\_handler(), RecastModel::nonlinear\_Resp\_Mapping, RecastModel::nonlinear\_Vars\_Mapping, RecastModel::primary\_Resp\_Map\_Indices, RecastModel::primary\_Resp\_Mapping, RecastModel::resp\_Mapping, RecastModel::secondary\_Resp\_Map\_Indices, RecastModel::secondary\_Resp\_Mapping, RecastModel::set\_Mapping, RecastModel::variables\_Mapping, and RecastModel::vars\_Map\_Indices.

Referenced by NonD\_Global\_Interval::core\_run(), NonD\_Local\_Interval::core\_run(), Data\_Transform\_Model::Data\_Transform\_Model(), Random\_Field\_Model::initialize\_recast(), Adapted\_Basis\_Model::initialize\_recast(), Active\_Subspace\_Model::initialize\_recast(), Eff\_Global\_Minimizer::minimize\_surrogates\_on\_model(), NonD\_Local\_Reliability::mpp\_search(), NonD\_Global\_Reliability::optimize\_gaussian\_process(), Probability\_Transform\_Model::Probability\_Transform\_Model(), and Scaling\_Model::Scaling\_Model().
void derived_evaluate ( const ActiveSet & set ) [protected], [virtual]

portion of evaluate() specific to RecastModel (forward to subModel.evaluate())

The RecastModel is evaluated by an Iterator for a recast problem formulation. Therefore, the currentVariables, incoming active set, and output currentResponse all correspond to the recast inputs/outputs.

Reimplemented from Model.

References Response::active_set(), Model::current_response(), Model::current_variables(), Model::currentResponse, Model::currentVariables, Model::evaluate(), RecastModel::recastModelEvalCtr, RecastModel::respMapping, RecastModel::subModel, RecastModel::transform_response(), RecastModel::transform_set(), RecastModel::transform_variables(), and Response::update().

Referenced by AdaptedBasisModel::derived_evaluate(), DataTransformModel::derived_evaluate(), ActiveSubspaceModel::derived_evaluate(), and RandomFieldModel::derived_evaluate().

void eval_tag_prefix ( const String & eval_id_str ) [inline], [protected], [virtual]

set the hierarchical eval ID tag prefix

RecastModel just forwards any tags to its subModel

Reimplemented from Model.

References Model::eval_tag_prefix(), and RecastModel::subModel.

void update_from_sub_model ( ) [private]

update current variables/labels/bounds/targets from subModel

Update inactive values and labels in currentVariables and inactive bound constraints in userDefinedConstraints from variables and constraints data within subModel.

References Model::aleatDistParams, Model::aleatory_distribution_parameters(), Constraints::continuous_lower_bounds(), Model::continuous_lower_bounds(), Constraints::continuous_upper_bounds(), Model::continuous_upper_bounds(), Variables::continuous_variable_labels(), Model::continuous_variable_labels(), Variables::continuous_variables(), Model::continuous_variables(), Model::current_variables(), Model::currentResponse, Model::currentVariables, Model::currentResponse, Model::currentVariables, Model::evaluate(), RecastModel::recastModelEvalCtr, RecastModel::respMapping, RecastModel::subModel, RecastModel::transform_response(), RecastModel::transform_set(), RecastModel::transform_variables(), and Response::update().

Referenced by AdaptedBasisModel::derived_evaluate(), DataTransformModel::derived_evaluate(), ActiveSubspaceModel::derived_evaluate(), and RandomFieldModel::derived_evaluate().
13.160 REDUCEDBASIS CLASS REFERENCE

Model::linear_ineq_constraint_coeffs(), Constraints::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_upper_bounds(), Constraints::linear_ineq_constraint_lower_bounds(), Constraints::nonlinear_eq_constraint_targets(), Model::nonlinear_eq_constraint_targets(), Constraints::nonlinear_ineq_constraint_upper_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Model::num_functions(), Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), Constraints::num_nonlinear_eq_constraints(), Constraints::num_nonlinear_ineq_constraints(), Model::numFns, Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Model::primaryRespFnSense, Model::primaryRespFnWts, RecastModel::primaryRespMapping, Model::response_labels(), RecastModel::secondaryRespMapping, Response::shared_data(), RecastModel::subModel, Model::userDefinedConstraints, and RecastModel::variablesMapping.

Referenced by RecastModel::update_from_subordinate_model().

The documentation for this class was generated from the following files:

- RecastModel.hpp
- RecastModel.cpp

13.160 ReducedBasis Class Reference

Public Member Functions

- ReducedBasis ()
  
  *default constructor*

- void set_matrix (const RealMatrix &)
- const RealMatrix & get_matrix ()
- void center_matrix ()
  
  *center the matrix by scaling each column by its means*

- void update_svd (bool center_matrix_by_col_means=true)
  
  *ensure that the factorization is current, centering if requested*

- bool is_valid () const
- const Real & get_singular_values_sum () const
- const Real & get_eigen_values_sum () const
- const RealVector & get_column_means ()
- const RealVector & get_singular_values () const
- RealVector get_singular_values (const TruncationCondition &)
- const RealMatrix & get_left_singular_vector ()
  
  *the num_observations n x num_observations n orthogonal matrix U; the left singular vectors are the first min(n,p) columns*

- const RealMatrix & get_right_singular_vectorTranspose () const
  
  *the num_responses p x num_responses p orthogonal matrix V'; the right singular vectors are the first min(n,p) rows of V' (columns of V)*

Private Attributes

- RealMatrix matrix
- RealMatrix workingMatrix
- RealMatrix U_matrix
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- RealVector S_values
- RealMatrix VT_matrix
- RealVector column_means
- bool col_means_computed
- bool is_centered
- bool is_valid_svd
- Real singular_values_sum
- Real eigen_values_sum
- TruncationCondition * truncation

13.160.1 Detailed Description

The ReducedBasis class is used to ... (TODO - RWH)

Class to manage data-driven dimension reduction. The passed matrix with num_observations n rows and num_responses p columns contains realizations of a set of responses. The class optionally centers the matrix by the column means. Stores a singular value decomposition of the passed data matrix X = U*S*V', which can also be used for PCA, where we seek an eigendecomposition of the covariance: X'*X = V*D*V'{-1} = V*S^2*V'^

The documentation for this class was generated from the following files:

- ReducedBasis.hpp
- ReducedBasis.cpp

13.161 RelaxedVarConstraints Class Reference

Derived class within the Constraints hierarchy which employs relaxation of discrete variables.

Inheritance diagram for RelaxedVarConstraints:

```
Constraints
|
RelaxedVarConstraints
```

Public Member Functions

- RelaxedVarConstraints (const SharedVariablesData &svd)
  lightweight constructor
- RelaxedVarConstraints (const ProblemDescDB &problem_db, const SharedVariablesData &svd)
  standard constructor
- ~RelaxedVarConstraints ()
  destructor
- void write (std::ostream &s) const
  write a variable constraints object to an std::ostream
- void read (std::istream &s)
  read a variable constraints object from an std::istream
13.162. RELAXEDVARIABLES CLASS REFERENCE

Additional Inherited Members

13.161.1 Detailed Description

Derived class within the Constraints hierarchy which employs relaxation of discrete variables.

Derived variable constraints classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The RelaxedVarConstraints derived class combines continuous and discrete domain types through integer relaxation. The branch and bound method uses this approach (see Variables::get_variables(problem_db) for variables type selection; variables type is passed to the Constraints constructor in Model).

13.161.2 Constructor & Destructor Documentation

RelaxedVarConstraints ( const ProblemDescDB & problem_db, const SharedVariablesData & svd )

standard constructor

In this class, a relaxed data approach is used in which continuous and discrete arrays are combined into a single continuous array (integrality is relaxed; the converse of truncating reals is not currently supported but could be in the future if needed). Iterators which use this class include: BranchBndOptimizer.

References

SharedVariablesData::all_relaxed_discrete_int(), SharedVariablesData::all_relaxed_discrete_real(), Constraints::allContinuousLowerBnds, Constraints::allContinuousUpperBnds, Constraints::allDiscreteIntLowerBnds, Constraints::allDiscreteIntUpperBnds, Constraints::allDiscreteRealLowerBnds, Constraints::allDiscreteRealUpperBnds, Dakota::copy_data_partial(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), Constraints::sharedVarsData, and SharedVariablesData::view().

The documentation for this class was generated from the following files:

- RelaxedVarConstraints.hpp
- RelaxedVarConstraints.cpp

13.162 RelaxedVariables Class Reference

Derived class within the Variables hierarchy which employs the relaxation of discrete variables.

Inheritance diagram for RelaxedVariables:

```
    Variables
     |
     v
     RelaxedVariables
```

Public Member Functions

- RelaxedVariables ( const ProblemDescDB & problem_db, const std::pair< short, short > & view )

    standard constructor

- RelaxedVariables ( const SharedVariablesData & svd )

    lightweight constructor

- ~RelaxedVariables ()

    destructor
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Protected Member Functions

- void read (std::istream &s)
  read a variables object from an std::istream

- void write (std::ostream &s, unsigned short vars_part=ALL_VARS) const
  write a variables object to an std::ostream, e.g., the console, optionally specifying which partition (all/active/inactive)

- void write_aprepro (std::ostream &s) const
  write a variables object to an std::ostream in aprepro format, e.g., a parameters file

- void read_tabular (std::istream &s, unsigned short vars_part=ALL_VARS)

- void write_tabular (std::ostream &s, unsigned short vars_part=ALL_VARS) const
  write a variables object in tabular format to an std::ostream, optionally specifying which partition (all/active/inactive)

- void write_tabular_labels (std::ostream &s, unsigned short vars_part=ALL_VARS) const
  write the labels in input spec order to a std::ostream, optionally specifying which partition (all/active/inactive)

- template<typename Reader >
  void read_core (std::istream &s, Reader read_handler, unsigned short vars_part)
  Implementation of reading various formats using the specified read handler, accounting for reordering due to relaxation.

- template<typename Writer >
  void write_core (std::ostream &s, Writer write_handler, unsigned short vars_part) const
  Implementation of writing various formats using the specified write handler, accounting for reordering due to relaxation.

Additional Inherited Members

13.162.1 Detailed Description

Derived class within the Variables hierarchy which employs the relaxation of discrete variables.

Derived variables classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The RelaxedVariables derived class combines continuous and discrete domain types but separates design, uncertain, and state variable types. The branch and bound method uses this approach (see Variables::get_variables(problem_db)).

13.162.2 Constructor & Destructor Documentation

RelaxedVariables ( const ProblemDescDB & problem_db, const std::pair< short, short > & view )

standard constructor

In this class, a relaxed data approach is used in which continuous and discrete arrays are combined into a single continuous array (integrality is relaxed; the converse of truncating reals is not currently supported but could be in the future if needed). Iterators/strategies which use this class include: BranchBndOptimizer. Extract fundamental variable types and labels and merge continuous and discrete domains to create aggregate arrays and views.

References SharedVariablesData::all_relaxed_discrete_int(), SharedVariablesData::all_relaxed_discrete_real(), Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, Dakota::copy_data_partial(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), ProblemDescDB::get_sa(), Variables::sharedVarsData, and SharedVariablesData::view().
13.163. RESPONSE CLASS REFERENCE

13.162.3 Member Function Documentation

void read tabular ( std::istream & s, unsigned short vars_part = ALL_VARS ) [protected], [virtual]
Presumes variables object is appropriately sized to receive data
  Reimplemented from Variables.
  References RelaxedVariables::read_core().

void read_core ( std::istream & s, Reader read_handler, unsigned short vars_part ) [protected]
Implementation of reading various formats using the specified read handler, accounting for reordering due to relaxation.
  Reordering is required in all read/write cases that will be visible to the user since all derived vars classes should use the same ordering for clarity. Neutral file I/O, binary streams, and packed buffers do not need to reorder (so long as read/write are consistent) since this data is not intended for public consumption.
  References SharedVariablesData::active_components_totals(), Variables::all_continuous_variable_labels(), Variables::all_discrete_int_variable_labels(), Variables::all_discrete_real_variable_labels(), Variables::all_discrete_string_variable_labels(), SharedVariablesData::all_relaxed_discrete_int(), SharedVariablesData::all_relaxed_discrete_real(), Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, SharedVariablesData::components_totals(), SharedVariablesData::cv_start(), SharedVariablesData::div_start(), SharedVariablesData::drv_start(), SharedVariablesData::dsv_start(), SharedVariablesData::icv_start(), SharedVariablesData::idrv_start(), SharedVariablesData::idsv_start(), SharedVariablesData::idiv_start(), SharedVariablesData::inactive_components_totals(), and Variables::sharedVarsData.
  Referenced by RelaxedVariables::read(), and RelaxedVariables::read_tabular().
  The documentation for this class was generated from the following files:
  • RelaxedVariables.hpp
  • RelaxedVariables.cpp

13.163 Response Class Reference

Container class for response functions and their derivatives. Response provides the enveloper base class.
  Inheritance diagram for Response:

```
          Response
         /    \
ExperimentResponse  SimulationResponse
```

Public Member Functions

- **Response ()**
  default constructor

- **Response (short type, const Variables &vars, const ProblemDescDB &problem_db)**
  standard constructor built from problem description database

- **Response (const SharedResponseData &srd, const ActiveSet &set)**
  alternate constructor that shares response data
• **Response** (short type, const `ActiveSet` &set)
  
  alternate constructor using limited data without sharing

• **Response** (const `SharedResponseData` &srd)
  
  alternate constructor using limited data (explicit disallows implicit type conversion)

• **Response** (const `Response` &response)
  
  copy constructor

• virtual `~Response` ()
  
  destructor

• **Response operator=** (const `Response` &response)
  
  assignment operator

• const `SharedResponseData` & `shared_data` () const
  
  return sharedRespData

• `SharedResponseData` & `shared_data` ()
  
  return sharedRespData

• `size_t num_functions` () const
  
  return the number of response functions

• const `ActiveSet` & `active_set` () const
  
  return the active set

• void `active_set` (const `ActiveSet` &set)
  
  set the active set

• const `ShortArray` & `active_set_request_vector` () const
  
  return the active set request vector

• void `active_set_request_vector` (const `ShortArray` &asrv)
  
  set the active set request vector and verify consistent number of response functions

• const `SizetArray` & `active_set_derivative_vector` () const
  
  return the active set derivative vector

• void `active_set_derivative_vector` (const `SizetArray` &asdv)
  
  set the active set derivative vector and reshape `functionGradients`/`functionHessians` if needed

• const `Real` & `function_value` (size_t `i`) const
  
  return a function value

• `Real` & `function_value_view` (size_t `i`)
  
  return a "view" of a function value for updating in place

• const `RealVector` & `function_values` () const
  
  return all function values

• `RealVector` `function_values_view` ()
  
  return all function values as a view for updating in place

• `RealVector` `function_values_view` () const
  
  return all function values as a view for accessing the function values vector from a const response

• void `function_value` (const `Real` &function_val, size_t `i`)
  
  set a function value

• void `function_values` (const `RealVector` &function_vals)
  
  set all function values

• const `Real` * `function_gradient` (int `i`) const
13.163. RESPONSE CLASS REFERENCE

- \texttt{return the i-th function gradient as a const Real\*}
  - RealVector \texttt{function\_gradient\_view (int i)}
    - \texttt{return the i-th function gradient as a SerialDenseVector view (shallow copy) for updating in place}
  - RealVector \texttt{function\_gradient\_view (int i) const}
    - \texttt{return the i-th function gradient as a SerialDenseVector view (shallow copy) for accessing a column vector from a const matrix}
  - RealVector \texttt{function\_gradient\_copy (int i) const}
    - \texttt{return the i-th function gradient as a SerialDenseVector Teuchos::Copy (deep copy)}
- \texttt{const RealMatrix & function\_gradients () const}
  - \texttt{return all function gradients}
  - RealMatrix \texttt{function\_gradients\_view ()}
    - \texttt{return all function gradients as a view for updating in place}
  - RealMatrix \texttt{function\_gradients\_view () const}
    - \texttt{return all function gradients as a view for updating in place}
  - void \texttt{function\_gradient (const RealVector &function\_grad, int i)}
    - \texttt{set a function gradient}
  - void \texttt{function\_gradients (const RealMatrix &function\_grads)}
    - \texttt{set all function gradients}
  - \texttt{const RealSymMatrix & function\_hessian (size\_t i) const}
    - \texttt{return the i-th function Hessian}
  - RealSymMatrix \texttt{function\_hessian\_view (size\_t i)}
    - \texttt{return the i-th function Hessian as a Teuchos::View (shallow copy) for updating in place}
  - RealSymMatrix \texttt{function\_hessian\_view (size\_t i) const}
    - \texttt{return the i-th function Hessian as a Teuchos::View (shallow copy) for accessing the i-th matrix within a const matrix array}
  - \texttt{const RealSymMatrixArray & function\_hessians () const}
    - \texttt{return all function Hessians}
  - RealSymMatrixArray \texttt{function\_hessians\_view ()}
    - \texttt{return all function Hessians as Teuchos::Views (shallow copies) for updating in place}
  - RealSymMatrixArray \texttt{function\_hessians\_view () const}
    - \texttt{return all function Hessians as Teuchos::Views (shallow copies) for updating in place}
  - void \texttt{function\_hessian (const RealSymMatrix &function\_hessian, size\_t i)}
    - \texttt{set a function Hessian}
  - void \texttt{function\_hessians (const RealSymMatrixArray &function\_hessians)}
    - \texttt{set all function Hessians}
- \texttt{RealVector field\_values\_view (size\_t i) const}
  - \texttt{return const field values}
  - RealVector \texttt{field\_values\_view (size\_t i)}
    - \texttt{return a "view" of a field value for updating in place}
  - void \texttt{field\_values (const RealVector &field\_val, size\_t i)}
    - \texttt{set a field value}
  - RealMatrix \texttt{field\_coords\_view (size\_t i)}
    - \texttt{return a "view" of a field value’s coordinates}
const RealMatrix field_coords_view (size_t i) const
return a const "view" of a field value's coordinates

void field_coords (const RealMatrix &field_coords, size_t i)
set a field value’s coordinates

RealMatrix field_gradients_view (size_t i) const
return a view of the gradients of each field element

RealSymMatrixArray field_hessians_view (size_t i) const
return a view of the hessians of each field element

const IntVector & field_lengths () const
return the field lengths from sharedRespData

void field_lengths (const IntVector &field_lens)
set the field lengths within sharedRespData

const IntVector & num_coords_per_field () const
return the num_coords_per_field from sharedRespData

void set_coord_values (const RealMatrix &coord_values, const size_t i)
set the coordinate values per field

const RealMatrix & get_coord_values (const size_t i) const
return the coordinate values per field

const StringArray & function_labels () const
return the fine-grained (unrolled) response function identifier strings from sharedRespData

void function_labels (const StringArray &labels)
set the fine-grained (unrolled) response function identifier strings within sharedRespData

const StringArray & field_group_labels ()
return the user-provided field group labels instead of the unrolled labels available through function_labels()

void read (std::istream &s, const unsigned short format=FLEXIBLE_RESULTS)
read a response object of specified format from an std::istream

void write (std::ostream &s) const
write a response object to an std::ostream

void read_annotated (std::istream &s)
read a response object in annotated format from an std::istream

void write_annotated (std::ostream &s) const
write a response object in annotated format to an std::ostream

void read_tabular (std::istream &s)
read responseRep::functionValues in tabular format from an std::istream

void write_tabular (std::ostream &s) const
write responseRep::functionValues in tabular format to an std::ostream

void write_tabular_labels (std::ostream &s) const
write the labels to a tabular data stream

void read (MPIUnpackBuffer &s)
read a response object from a packed MPI buffer

void write (MPIPackBuffer &s) const
write a response object to a packed MPI buffer

Response copy (bool deep_srd=false) const
return a deep response copy of the contained responseRep for use in history mechanisms (SharedResponseData uses a shallow copy by default)

- int data_size ()
  return the number of doubles active in response. Used for sizing double* response data arrays passed into read_data and write_data.

- void read_data (double *response_data)
  read from an incoming double* array

- void write_data (double *response_data)
  write to an incoming double* array

- void overlay (const Response &response)
  add incoming response to functionValues/Gradients/Hessians

- void update (const Response &response)
  Used in place of operator= when only results data updates are desired (functionValues/functionGradients/function-Hessians are updated, ASV/labels/id's/etc. are not). Care is taken to allow different derivative array sizing between the two response objects.

- void update (const RealVector &source_fn_vals, const RealMatrix &source_fn_grads, const RealSymMatrixArray &source_fn_hessians, const ActiveSet &source_set)
  Overloaded form which allows update from components of a response object. Care is taken to allow different derivative array sizing.

- void update_partial (size_t start_index_target, size_t num_items, const Response &response, size_t start_index_source)
  partial update of this response object from another response object. The response objects may have different numbers of response functions.

- void update_partial (size_t start_index_target, size_t num_items, const RealVector &source_fn_vals, const RealMatrix &source_fn_grads, const RealSymMatrixArray &source_fn_hessians, const ActiveSet &source_set, size_t start_index_source)
  Overloaded form which allows partial update from components of a response object. The response objects may have different numbers of response functions.

- void reshape (size_t num_fns, size_t num_params, bool grad_flag, bool hess_flag)
  reshapes response data arrays

- void reset ()
  resets all response data to zero

- void reset_inactive ()
  resets all inactive response data to zero

- bool is_null () const
  function to check responseRep (does this handle contain a body)

- virtual void set_scalar_covariance (RealVector &scalars)
  method to set the covariance matrix defined for ExperimentResponse

- virtual const ExperimentCovariance & experiment_covariance () const
  retrieve the ExperimentCovariance structure

- virtual void set_full_covariance (std::vector<RealMatrix> &matrices, std::vector<RealVector> &diagonals, RealVector &scalars, IntVector matrix_map_indices, IntVector diagonal_map_indices, IntVector scalar_map_indices)
  method to set the full covariance matrices for ExperimentResponse
• virtual Real apply_covariance (const RealVector &residuals) const
  method to compute the triple product $v'\cdot\text{inv}(C)\cdot v$.
• virtual void apply_covariance_inv_sqrt (const RealVector &residuals, RealVector &weighted_residuals) const
  method to compute $(v'\cdot\text{inv}(C))^{1/2}$, to compute weighted residual
• virtual void apply_covariance_inv_sqrt (const RealMatrix &gradients, RealMatrix &weighted_gradients) const
• virtual void apply_covariance_inv_sqrt (const RealSymMatrixArray &hessians, RealSymMatrixArray &weighted_hessians) const
• virtual void get_covariance_diagonal (RealVector &diagonal) const
• virtual Real covariance_determinant () const
covariance determinant for one experiment (default 1.0)
• virtual Real log_covariance_determinant () const
  log of covariance determinant for one experiment (default 0.0)

Protected Member Functions

• Response (BaseConstructor, const Variables &vars, const ProblemDescDB &problem_db)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
• Response (BaseConstructor, const SharedResponseData &srd, const ActiveSet &set)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
• Response (BaseConstructor, const ActiveSet &set)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
• Response (BaseConstructor, const SharedResponseData &srd)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
• virtual void copy_rep (Response *source_rep)
  Implementation of data copy for Response letters (specialized by some derived letter types); pulls base class data from source_rep into the this object.

Protected Attributes

• SharedResponseData sharedRespData
  reference-counted instance of shared response data: id’s, labels
• RealVector functionValues
  abstract set of response functions
• RealMatrix functionGradients
  first derivatives of the response functions
• RealSymMatrixArray functionHessians
  second derivatives of the response functions
• IntRealMatrixMap fieldCoords
  coordinates for the field values
• ActiveSet responseActiveSet
  copy of the ActiveSet used by the Model to generate a Response instance
Private Member Functions

- template<class Archive , typename OrdinalType , typename ScalarType >
  void write_sdm_col (Archive &ar, int col, const Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm) const
  write a column of a SerialDenseMatrix
- template<class Archive , typename OrdinalType , typename ScalarType >
  void read_sdm_col (Archive &ar, int col, Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm)
  read a column of a SerialDenseMatrix
- template<class Archive >
  void load (Archive &ar, const unsigned int version)
  read a Response from an archive
- template<class Archive >
  void load_rep (Archive &ar, const unsigned int version)
  read a Response letter object from an archive
- template<class Archive >
  void save (Archive &ar, const unsigned int version) const
  write a Response to an archive
- template<class Archive >
  void save_rep (Archive &ar, const unsigned int version) const
  write a Response letter object to an archive
- BOOST_SERIALIZATION_SPLIT_MEMBER ()
  Response * get_response(short type)
  Used by standard envelope constructor to instantiate a new letter class.
- Response * get_response (const SharedResponseData &srd, const ActiveSet &set) const
  Used by alternate envelope constructor to instantiate a new letter class.
- Response * get_response (short type, const ActiveSet &set) const
  Used by alternate envelope constructor to instantiate a new letter class.
- Response * get_response (const SharedResponseData &srd) const
  Used by copy() to instantiate a new letter class.
- Response * get_response (short type) const
  Used by read functions to instantiate a new letter class.
- void read_annotated_rep (std::istream &s)
  read a letter object in annotated format from an std::istream
- void write_annotated_rep (std::ostream &s) const
  write a letter object in annotated format to an std::ostream
- void read_rep (MPIUnpackBuffer &s)
  read a letter object from a packed MPI buffer
- void write_rep (MPIPackBuffer &s) const
  write a letter object to a packed MPI buffer
- void shape_rep (const ActiveSet &set, bool initialize=true)
  resizes the representation’s containers
- void reshape_rep (size_t num_fns, size_t num_params, bool grad_flag, bool hess_flag)
  resizes the representation’s containers
- void read_gradients (std::istream &s, const ShortArray &asv, std::ostream &error)
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Read gradients from a freeform stream. Insert error messages.
• void read_hessians (std::istream &s, const ShortArray &asv, std::ostringstream &error)
  Read Hessians from a freeform stream. Insert error messages.
• void read_labeled_fn_vals (std::istream &s, const ShortArray &asv, std::ostringstream &errors)
  Read function values from an annotated stream. Insert error messages.
• void read_flexible_fn_vals (std::istream &s, const ShortArray &asv, std::ostringstream &errors)
  Read function values from a stream in a "flexible" way – ignoring any labels. Insert error messages into errors stream.
• bool failure_reported (std::istream &s)
  Check for FAIL in stream.

Private Attributes
• const Variables & vars
• const Variables const
  ProblemDescDB &problem_db const
• Response * responseRep
  pointer to the body (handle-body idiom)
• int referenceCount
  number of handle objects sharing responseRep

Friends
• class boost::serialization::access
• bool operator==(const Response &resp1, const Response &resp2)
  equality operator
• bool operator!=(const Response &resp1, const Response &resp2)
  inequality operator

13.163.1 Detailed Description
Container class for response functions and their derivatives. Response provides the enveloper base class.

The Response class is a container class for an abstract set of functions (functionValues) and their first (function-Gradients) and second (functionHessians) derivatives. The functions may involve objective and constraint functions (optimization data set), least squares terms (parameter estimation data set), or generic response functions (uncertainty quantification data set). For memory efficiency, it employs the "letter-envelope idiom" approach to reference counting and representation sharing (see Coplien "Advanced C++"), for which the base Response class serves as the envelope and one of its derived classes serves as the letter.

13.163.2 Member Data Documentation

RealMatrix functionGradients [protected]
first derivatives of the response functions
  the gradient vectors (plural) are column vectors in the matrix (singular) with (row, col) = (variable index, response fn index).
Referenced by Response::field_gradients_view(), Response::function_gradient(), Response::function_gradient_copy(), Response::function_gradient_view(), Response::function_gradients(), and Response::function_gradients_view().

The documentation for this class was generated from the following file:

- DakotaResponse.hpp

### 13.164 RestartWriter Class Reference

#### Public Member Functions

- **RestartWriter ()**
  
  *optional default ctor allowing a non-outputting RestartWriter*

- **RestartWriter (const String &write_restart_filename)**
  
  *typical ctor taking a filename*

- **const String & filename ()**
  
  *output filename for this writer*

- **void append_prp (const ParamResponsePair &prp_in)**
  
  *add the passed pair to the restart file*

- **void flush ()**
  
  *flush the restart stream so we have a complete restart record should Dakota abort*

#### Private Member Functions

- **RestartWriter (const RestartWriter &)**
  
  *copy constructor is disallowed due to file stream*

- **const RestartWriter & operator= (const RestartWriter &)**
  
  *assignment is disallowed due to file stream*

#### Private Attributes

- **String restartOutputFilename**
  
  *the name of the restart output file*

- **std::ofstream restartOutputFS**
  
  *Binary stream to which restart data is written.*

- **boost::scoped_ptr < boost::archive::binary_oarchive > restartOutputArchive**
  
  *Binary output archive to which data is written (pointer since no default ctor for oarchive and may not be initialized).*

### 13.164.1 Detailed Description

Component for writing restart files. Creation and destruction of archive and associated stream are managed here.

The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp
13.165 ResultsDBAny Class Reference

Public Member Functions

- template<
typename StoredType >
  void array_allocate (const StrStrSizet &iterator_id, const std::string &data_name, size_t array_size, const MetaDataType &metadata)

  allocate an entry with sized array of the StoredType, e.g., array across response functions or optimization results sets

- template<
typename StoredType >
  void array_insert (const StrStrSizet &iterator_id, const std::string &data_name, size_t index, const StoredType &sent_data)

  insert sent_data in specified position in previously allocated array

- template<
typename StoredType >
  StoredType get_data (const StrStrSizet &iterator_id, const std::string &data_name) const

  return requested data by value in StoredType

- template<
typename StoredType >
  StoredType get_array_data (const StrStrSizet &iterator_id, const std::string &data_name, size_t index) const

  return requested data from array by value in StoredType

- template<
typename StoredType >
  const StoredType * get_data_ptr (const StrStrSizet &iterator_id, const std::string &result_key) const

  return pointer to stored data entry

- template<
typename StoredType >
  const StoredType * get_array_data_ptr (const StrStrSizet &iterator_id, const std::string &data_name, size_t index) const

  return pointer to stored data at given array location

- void insert (const StrStrSizet &iterator_id, const std::string &data_name, const boost::any &result, const MetaDataType &metadata)

  record addition with metadata map

- void dump_data (std::ostream &output_stream)

  coarsely dump the data to the passed output stream

- void print_data (std::ostream &output_stream)

  pretty print the data to the passed output stream

Private Member Functions

- const ResultsValueType & lookup_data (const StrStrSizet &iterator_id, const std::string &data_name) const

  attempt to find the requested data, erroring if not found

- template<
typename StoredType >
  StoredType cast_data (const boost::any &dataholder) const

  cast the reference to the any data to the requested type

- template<
typename StoredType >
  const StoredType * cast_data_ptr (const boost::any *dataholder) const

  cast the pointer to the any data to the requested type
• void `print_metadata` (std::ostream &os, const MetaDataType &md)
  print metadata to ostream
• void `extract_data` (const boost::any &dataholder, std::ostream &os)
  determine the type of contained data and output it to ostream
• void `output_data` (const std::vector<double> &data, std::ostream &os)
  output data to ostream
• void `output_data` (const std::vector<RealVector> &data, std::ostream &os)
  output data to ostream
• void `output_data` (const std::vector<std::string> &data, std::ostream &os)
  output data to ostream
• void `output_data` (const std::vector<std::vector<std::string>> &data, std::ostream &os)
  output data to ostream
• void `output_data` (const std::vector<RealMatrix> &data, std::ostream &os)
  output data to ostream
• void `output_data` (const RealMatrix &data, std::ostream &os)
  output data to ostream

Private Attributes
• std::map< ResultsKeyType, ResultsValueType > iteratorData
  core data storage (map from key to value type)

13.165.1 Detailed Description
Class: ResultsDBAny Description: A map-based container to store DAKOTA Iterator results in underlying boost-::anys, with optional metadata

13.165.2 Member Function Documentation

`void array_insert` ( const StrStrSizet & iterator_id, const std::string & data_name, size_t index, const StoredType & sent_data )

insert sent_data in specified position in previously allocated array
  insert requires previous allocation, and does not allow metadata update
  References Dakota::abort_handler(), ResultsDBAny::iteratorData, and Dakota::make_key().

`void insert` ( const StrStrSizet & iterator_id, const std::string & data_name, const boost::any & result, const MetaDataType & metadata )

record addition with metadata map
  Add or update existing entry
  References ResultsDBAny::iteratorData, and Dakota::make_key().
  Referenced by ResultsDBAny::array_allocate().
void extract_data ( const boost::any & dataholder, std::ostream & os ) [private]

determine the type of contained data and output it to ostream
   Extract the data from the held any and map to supported concrete types int double RealVector (Teuchos::-
   SerialDenseVector<int,double) RealMatrix (Teuchos::SerialDenseMatrix<int,double)
   References ResultsDBAny::output_data().
   Referenced by ResultsDBAny::dump_data(), and ResultsDBAny::print_data().
   The documentation for this class was generated from the following files:
   
   • ResultsDBAny.hpp
   • ResultsDBAny.cpp

13.166 ResultsEntry<StoredType> Class Template Reference

Class to manage in-core vs. file database lookups.

Public Member Functions

• ResultsEntry (const ResultsManager &results_mgr, const StrStrSizet &iterator_id, const std::string &data-
  name)
   Construct ResultsEntry containing retrieved item of StoredType.

• ResultsEntry (const ResultsManager &results_mgr, const StrStrSizet &iterator_id, const std::string &data-
  name, size_t array_index)
   Construct ResultsEntry to retrieve item array_index from array of StoredType.

Private Member Functions

• ResultsEntry ()
   return a reference to the stored data, whether from core or file

Private Attributes

• bool coreActive
   whether the ResultsManager has an active in-core database

• StoredType dbData
   data retrieved from file data base

• const StoredType * dbDataPtr
   non-const pointer to const data we don’t own in the core case

13.166.1 Detailed Description

template<typename StoredType> class Dakota::ResultsEntry<StoredType>

Class to manage in-core vs. file database lookups.
   ResultsEntry manages database lookups. If a core database is available, will return a reference directly to the
   stored data; if disk, will return reference to a local copy contained in this class. Allows disk-stored data to persist
   for minimum time during lookup to support true out-of-core use cases.
13.166.2 Constructor & Destructor Documentation

ResultsEntry( ) [private]

return a reference to the stored data, whether from core or file
default construction disallowed: data must be initialized from DB lookup if needed

The documentation for this class was generated from the following file:

- ResultsManager.hpp

13.167 ResultsFileError Class Reference

exception throw for other results file read error

The documentation for this class was generated from the following file:

- dakota_global_defs.hpp

13.167.1 Detailed Description

exception throw for other results file read error

The documentation for this class was generated from the following file:

- dakota_global_defs.hpp

13.168 ResultsID Class Reference

Get a globally unique 1-based execution number for a given iterator name (combination of methodName and methodID) for use in results DB. Each Iterator::run() call creates or increments this count for its string identifier.

Public Member Functions

- size_t increment_id (const std::string &methodName, const std::string &methodId) explicit increment the iterator results ID, init to 1 if needed
- size_t get_id (const std::string &methodName, const std::string &methodId) get (possibly creating) a unique iterator results ID for the passed name
- size_t get_id (const std::string &methodName, const std::string &methodId) const get a unique iterator results ID for the passed name (const version errors if not found)
Static Public Member Functions

- static ResultsID & instance ()
  
  get the single unique instance of ResultsID

Private Member Functions

- ResultsID ()
  
  Private constructor for ResultsID.
- ~ResultsID ()
  
  Private destructor for ResultsID.
- ResultsID (ResultsID const &)
  
  Private copy constructor for ResultsID.
- ResultsID & operator= (ResultsID const &)
  
  Private assignment operator for ResultsID.

Private Attributes

- std::map<std::pair<std::string, std::string>, size_t> idMap
  
  storage for the results IDs

13.168.1 Detailed Description

Get a globally unique 1-based execution number for a given iterator name (combination of methodName and methodID) for use in results DB. Each Iterator::run() call creates or increments this count for its string identifier.

The documentation for this class was generated from the following files:

- ResultsManager.hpp
- ResultsManager.cpp

13.169 ResultsManager Class Reference

Results manager for iterator final data.

Public Member Functions

- ResultsManager ()
  
  default constructor: no databases active until initialize called
- void initialize (const std::string &base_filename)
  
  initialize the results manager to manage an in-core database, writing to the specified file name
- bool active () const
  
  whether any databases are active
- void write_databases ()
  
  Write in-core databases to file.
template<typename StoredType>
void insert (const StrStrSizet &iterator_id, const std::string &data_name, const StoredType &sent_data, 
const MetaDataType metadata=MetaDataType())
insert data

void insert (const StrStrSizet &iterator_id, const std::string &data_name, StringMultiArrayConstView sma_labels, const MetaDataType metadata=MetaDataType())

template<typename StoredType>
void array_allocate (const StrStrSizet &iterator_id, const std::string &data_name, size_t array_size, const MetaDataType metadata=MetaDataType())
allocate an entry with array of StoredType of array_size for future insertion; likely move to non-templated accessors for these

template<typename StoredType>
void array_insert (const StrStrSizet &iterator_id, const std::string &data_name, size_t index, const StoredType &sent_data)
insert into a previously allocated array of StoredType at index specified; metadata must be specified at allocation

template<typename StoredType>
void array_insert (const StrStrSizet &iterator_id, const std::string &data_name, size_t index, StringMultiArrayConstView sent_data)
specialization: insert a SMACV into a previously allocated array of StringArrayStoredType at index specified; metadata must be specified at allocation

Public Attributes

• ResultsNames results_names
Copy of valid results names for when manager is passed around.

Private Member Functions

• template<typename StoredType>
StoredType core_lookup (const StrStrSizet &iterator_id, const std::string &data_name) const
retrieve in-core entry given by id and name

• template<typename StoredType>
StoredType * core_lookup_ptr (const StrStrSizet &iterator_id, const std::string &data_name) const
retrieve data via pointer to avoid copy; work-around for Boost any use of pointer (could use utilib::Any)

• template<typename StoredType>
StoredType core_lookup (const StrStrSizet &iterator_id, const std::string &data_name, size_t index) const
retrieve data from in-core array of StoredType at given index

• template<typename StoredType>
const StoredType * core_lookup_ptr (const StrStrSizet &iterator_id, const std::string &data_name, size_t index) const
retrieve data via pointer to entry in in-core array

• template<typename StoredType>
void file_lookup (StoredType &db_data, const StrStrSizet &iterator_id, const std::string &data_name) const
retrieve requested data into provided db_data StoredType
Private Attributes

- bool coreDBActive
  whether the in-core database is active
- std::string coreDBFilename
  filename for the in-core database
- bool hdf5DBActive
  whether the file database is active
- boost::scoped_ptr<ResultsDBAny> coreDB
  In-core database, with option to flush to file at end.
- boost::shared_ptr<ResultsDBHDF5> hdf5DB
  File-based database; using shared_ptr due to potentially incomplete type and requirements for checked_delete in debug builds.

Friends

- template<typename StoredType>
class ResultsEntry
  ResultsEntry is a friend of ResultsManager.

13.169.1 Detailed Description

Results manager for iterator final data.

The results manager provides the API for posting and retrieving iterator results data (and eventually run config/statistics). It can manage a set of underlying results databases, in or out of core, depending on configuration.

The key for a results entry is documented in results_types.hpp, e.g., tuple<std::string, std::string, size_t, std::string>

For now, using concrete types for most insertion, since underlying databases like HDF5 might need concrete types; though template parameter for array allocation and retrieval.

All insertions overwrite any previous data.

The documentation for this class was generated from the following files:

- ResultsManager.hpp
- ResultsManager.cpp

13.170 ResultsNames Class Reference

List of valid names for iterator results.

Public Member Functions

- ResultsNames ()
  Default constructor initializes all valid names.
13.170. RESULTSNAMES CLASS REFERENCE

Public Attributes

- `size_t namesVersion`
- `std::string best_cv`
- `std::string best_div`
- `std::string best_dsv`
- `std::string best_drv`
- `std::string best_fns`
- `std::string moments_std`
- `std::string moments_central`
- `std::string moments_std_num`
- `std::string moments_central_num`
- `std::string moments_std_exp`
- `std::string moments_central_exp`
- `std::string moment_cis`
- `std::string extreme_values`
- `std::string map_resp_prob`
- `std::string map_resp_rel`
- `std::string map_resp_genrel`
- `std::string map_prob_resp`
- `std::string map_rel_resp`
- `std::string map_genrel_resp`
- `std::string pdf_histograms`
- `std::string correl_simple_all`
- `std::string correl_simple_io`
- `std::string correl_partial_io`
- `std::string correl_simple_rank_all`
- `std::string correl_simple_rank_io`
- `std::string correl_partial_rank_io`
- `std::string pce_coeffs`
- `std::string pce_coeff_labels`
- `std::string cv_labels`
- `std::string div_labels`
- `std::string dsv_labels`
- `std::string drv_labels`
- `std::string fn_labels`

13.170.1 Detailed Description

List of valid names for iterator results.

All data in the `ResultsNames` class is public, basically just a struct

The documentation for this class was generated from the following file:

- ResultsManager.hpp
13.171 RichExtrapVerification Class Reference

Class for Richardson extrapolation for code and solution verification.

Inheritance diagram for RichExtrapVerification:

```
    Iterator
     |
     V
    Analyzer
     |
     V
    Verification
     |
   RichExtrapVerification
```

Public Member Functions

- `RichExtrapVerification (ProblemDescDB &problem_db, Model &model)`
  constructor
- `~RichExtrapVerification ()`
  destructor
- `void core_run ()`
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- `void print_results (std::ostream &s)`
  print the final iterator results

Private Member Functions

- `void estimate_order ()`
  perform a single estimation of convOrder using extrapolation()
- `void converge_order ()`
  iterate using extrapolation() until convOrder stabilizes
- `void converge_qoi ()`
  iterate using extrapolation() until QOIs stabilize
- `void extrapolation (const RealVector &refine_triple, RealMatrix &qoi_triples)`
  estimate convOrder from refinement and quantity of interest (QOI) triples
- `void extrapolate_result (const RealVector &refine_triple, const RealMatrix &qoi_triples)`
  predict the converged value based on the convergence rate and the value of Phi

Private Attributes

- `unsigned short studyType`
  internal code for extrapolation study type: SUBMETHOD_{CONVERGE_ORDER,CONVERGE_QOI,ESTIMATE_ORDER}
- `size_t numFactors`
number of refinement factors defined from active state variables

- RealVector initialCVars
  initial reference values for refinement factors

- size_t factorIndex
  the index of the active factor

- Real refinementRate
  rate of mesh refinement (default = 2.)

- RealMatrix convOrder
  the orders of convergence of the QOIs (numFunctions by numFactors)

- RealMatrix extrapQOI
  the extrapolated value of the QOI (numFunctions by numFactors)

- RealMatrix numErrorQOI
  the numerical uncertainty associated with level of refinement (numFunctions by numFactors)

- RealVector refinementRefPt
  This is a reference point reported for the converged extrapQOI and numErrorQOI. It currently corresponds to the coarsest mesh in the final refinement triple.

Additional Inherited Members

13.171.1 Detailed Description

Class for Richardson extrapolation for code and solution verification.

The RichExtrapVerification class contains several algorithms for performing Richardson extrapolation.

13.171.2 Member Function Documentation

void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Dakota::abort_handler(), Model::continuous_variables(), RichExtrapVerification::converge_order(),
RichExtrapVerification::converge_qoi(), RichExtrapVerification::convOrder, RichExtrapVerification::estimate_order(),
RichExtrapVerification::extrapQOI, RichExtrapVerification::initialCVars, Iterator::iteratedModel, RichExtrapVerification-
::numErrorQOI, RichExtrapVerification::numFactors, Analyzer::numFunctions, Iterator::outputLevel, RichExtrap-
Verification::refinementRefPt, and RichExtrapVerification::studyType.

void print_results ( std::ostream & s ) [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation
summary printed in finalize_run().

Reimplemented from Verification.

References Model::continuous_variable_labels(), RichExtrapVerification::convOrder, Dakota::copy_data(), Rich-
ExtrapVerification::extrapQOI, Iterator::iteratedModel, RichExtrapVerification::numErrorQOI, Verification::print-
_results(), RichExtrapVerification::refinementRate, RichExtrapVerification::refinementRefPt, and Model::response-
_labels().
**void estimate_order( ) [private]**

perform a single estimation of convOrder using extrapolation()

This algorithm executes a single refinement triple and returns convergence order estimates.


Referenced by RichExtrapVerification::core_run().

**void converge_order( ) [private]**

iterate using extrapolation() until convOrder stabilizes

This algorithm continues to refine until the convergence order estimate converges.


Referenced by RichExtrapVerification::core_run().

**void converge_qoi( ) [private]**

iterate using extrapolation() until QOIs stabilize

This algorithm continues to refine until the discretization error lies within a prescribed tolerance.


Referenced by RichExtrapVerification::core_run().

The documentation for this class was generated from the following files:

- RichExtrapVerification.hpp
- RichExtrapVerification.cpp

### 13.172 ScalingModel Class Reference

Scaling specialization of RecastModel.

Inheritance diagram for ScalingModel:

```
  Model
     
RecastModel
     
ScalingModel
```
Public Member Functions

- **ScalingModel (Model &sub_model)**
  
  *standard constructor*

- ~**ScalingModel ()**
  
  *destructor*

- **RealVector cv_scaled2native (const RealVector &scaled_cv) const**
  
  *Public members for help in final results recovery*

- **void resp_scaled2native (const Variables &native_vars, Response &updated_resp) const**
  
  *map responses from scaled to native space, updating provided Response in-place (on entry it’s scaled response, on exit it’s native)*

- **void secondary_resp_scaled2native (const RealVector &scaled_nln_cons, const ShortArray &asv, RealVector &native_fns) const**
  
  *Use scaled nonlinear constraints (sized total functions) to update the nonlinear constraints portion of the passed native_fns array.*

Protected Member Functions

- **void initialize_scaling (Model &sub_model)**
  
  *initialize scaling types, multipliers, and offsets; perform error checking*

- **void compute_scaling (int object_type, int auto_type, int num_vars, RealVector &lbs, RealVector &ubs, RealVector &targets, const StringArray &scale_strings, const RealVector &scales, IntArray &scale_types, RealVector &scale_mults, RealVector &scale_offsets)**
  
  *general helper function for initializing scaling types and factors on a vector of variables, functions, constraints, etc.*

- **RealMatrix lin_coeffs_modify_n2s (const RealMatrix &native_coeffs, const RealVector &cv_multipliers, const RealVector &lin_multipliers) const**
  
  *general linear coefficients mapping from native to scaled space*

- **bool compute_scale_factor (const Real lower_bound, const Real upper_bound, Real *multiplier, Real *offset)**
  
  *automatically compute a single scaling factor – bounds case*

- **bool compute_scale_factor (const Real target, Real *multiplier)**
  
  *automatically compute a single scaling factor – target case*

- **void print_scaling (const String &info, const IntArray &scale_types, const RealVector &scale_mults, const RealVector &scale_offsets, const StringArray &labels)**
  
  *print scaling information for a particular response type in tabular form*

- **bool need_resp_trans_byvars (const ShortArray &asv, int start_index, int num_resp) const**
  
  *determine if response transformation is needed due to variable transformations*

- **RealVector modify_n2s (const RealVector &native_vars, const IntArray &scale_types, const RealVector &multipliers, const RealVector &offsets) const**
  
  *general RealVector mapping from native to scaled variables vectors:*

- **RealVector modify_s2n (const RealVector &scaled_vars, const IntArray &scale_types, const RealVector &multipliers, const RealVector &offsets) const**
  
  *general RealVector mapping from scaled to native variables (and values)*

- **void response_modify_n2s (const Variables &scaled_vars, const Response &native_response, Response &scaled_response, int start_offset, int num_responses) const**
map responses from native to scaled variable space

- void response_modify_s2n (const Variables &native_vars, const Response &scaled_response, Response &native_response, int start_offset, int num_responses) const

  map responses from scaled to native space

Static Protected Member Functions

- static short response_order (const Model &sub_model)
  helper to compute the recast response order during member initialization
- static bool scaling_active (const StringArray &scale_types)
  check whether the passed scale strings include any active (!= none) scale types
- static void variables_scaler (const Variables &scaled_vars, Variables &native_vars)
  RecastModel callback for variables scaling: transform variables from scaled to native (user) space.
- static void variables_unscaler (const Variables &scaled_vars, Variables &native_vars)
  RecastModel callback for inverse variables scaling: transform variables from native (user) to scaled space.
- static void primary_resp_scaler (const Variables &native_vars, const Variables &scaled_vars, const Response &native_response, Response &iterator_response)
  RecastModel callback for primary response scaling: transform responses (grads, Hessians) from native (user) to scaled space.
- static void secondary_resp_scaler (const Variables &native_vars, const Variables &scaled_vars, const Response &native_response, Response &scaled_response)
  RecastModel callback for secondary response scaling: transform constraints (grads, Hessians) from native (user) to scaled space.

Protected Attributes

- bool varsScaleFlag
  flag for variables scaling
- bool primaryRespScaleFlag
  flag for primary response scaling
- bool secondaryRespScaleFlag
  flag for secondary response scaling
- IntArray cvScaleTypes
  scale flags for continuous vars.
- RealVector cvScaleMultipliers
  scales for continuous variables
- RealVector cvScaleOffsets
  offsets for continuous variables
- IntArray responseScaleTypes
  scale flags for all responses
- RealVector responseScaleMultipliers
  scales for all responses
- RealVector responseScaleOffsets
  offsets for all responses (zero < for functions, not for nonlin con)
13.172. SCALINGMODEL CLASS REFERENCE

- `IntArray linearIneqScaleTypes`
  
  scale flags for linear ineq

- `RealVector linearIneqScaleMultipliers`
  
  scales for linear ineq constrs.

- `RealVector linearIneqScaleOffsets`
  
  offsets for linear ineq constrs.

- `IntArray linearEqScaleTypes`
  
  scale flags for linear eq.

- `RealVector linearEqScaleMultipliers`
  
  scales for linear constraints

- `RealVector linearEqScaleOffsets`
  
  offsets for linear constraints

Static Protected Attributes

- static `ScalingModel * scaleModelInstance`
  
  static pointer to this class for use in static callbacks

Additional Inherited Members

13.172.1 Detailed Description

Scaling specialization of `RecastModel`.

Specialization of `RecastModel` to scale Variables and/or Responses This class provides a simple constructor that forwards to the more complicated `RecastModel` API

13.172.2 Constructor & Destructor Documentation

`ScalingModel ( Model & sub_model )`

standard constructor

This constructor computes various indices and mappings, then updates the properties of the `RecastModel` References `Model::cv()`, `ScalingModel::cvScaleTypes`, `Model::div()`, `Model::drv()`, `Model::dsv()`, `RecastModel::init_mapping()`, `ScalingModel::initialize_scaling()`, `RecastModel::inverse_mappings()`, `Model::num_functions()`, `Model::num_primary_fns()`, `Model::output_level`, `ScalingModel::primary_responder()`, `Model::primary_response_fn_sense()`, `Model::primary_response_fn_weights()`, `ScalingModel::primaryRespScaleFlag`, `ScalingModel::primaryRespScaleOffset`, `ScalingModel::primaryRespScaleScaling`, `ScalingModel::primaryRespScaleUnscaling`, `ScalingModel::primaryRespScaleFlag`, `ScalingModel::variables鳞atom()`, `ScalingModel::variables_unscaler()`, and `ScalingModel::varsScaleFlag`.  

13.172.3 Member Function Documentation

`RealVector cv_scaled2native ( const RealVector & scaled_cv ) const`

Public members for help in final results recovery

recover native variable values from the scaled space

Since this convenience function is public, it must have a fall-through to return a copy for when this scaling type isn’t active.
References ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, ScalingModel::modify_s2n(), and ScalingModel::varsScaleFlag.

Referenced by LeastSq::post_run(), and Optimizer::post_run().

```cpp
void resp_scaled2native ( const Variables & native_vars, Response & updated_resp ) const
```

map responses from scaled to native space, updating provided Response in-place (on entry it’s scaled response, on exit it’s native)

Since this convenience function is public, it must behave correctly when this scale type isn’t active. It does, because it modifies in-place

References Response::active_set_request_vector(), Response::copy(), ScalingModel::need_resp_trans_byvars(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), ScalingModel::primaryRespScaleFlag, ScalingModel::response_modify_s2n(), ScalingModel::secondaryRespScaleFlag, and Response::update_partial().

Referenced by LeastSq::post_run(), and Optimizer::post_run().

```cpp
void secondary_resp_scaled2native ( const RealVector & scaled_nln_cons, const ShortArray & asv, RealVector & native_fns ) const
```

Use scaled nonlinear constraints (sized total functions) to update the nonlinear constraints portion of the passed native_fns array.

Since this convenience function is public, it must have a fall-through to return a copy for when this scaling type isn’t active.

References Dakota::copy_data_partial(), ScalingModel::modify_s2n(), ScalingModel::need_resp_trans_byvars(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, ScalingModel::responseScaleTypes, and ScalingModel::secondaryRespScaleFlag.

```cpp
void initialize_scaling ( Model & sub_model ) [protected]
```

initialize scaling types, multipliers, and offsets; perform error checking

Initialize scaling types, multipliers, and offsets. Update the iteratedModel appropriately

References Dakota::abort_handler(), ScalingModel::compute_scaling(), Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variable_labels(), Model::continuous_variables(), Dakota::copy_data(), Model::cv(), ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, ScalingModel::lin_coeffs_modify_n2s(), Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_upper_bounds(), ScalingModel::linearEqScaleMultipliers, ScalingModel::linearEqScaleOffsets, ScalingModel::linearEqScaleTypes, Model::linearEqScaleMultipliers, ScalingModel::linearEqScaleOffsets, ScalingModel::linearEqScaleTypes, Model::modify_n2s(), Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Model::num_functions(), Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::outputLevel, ScalingModel::primaryRespScaleFlag, ScalingModel::print_scaling(), Model::response_labels(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, ScalingModel::responseScaleTypes, ScalingModel::scaling_active(), Model::scalingOpts, ScalingModel::secondaryRespScaleFlag, Model::supports_derivative_estimation(), Model::supports_EstimDerivs, and ScalingModel::varsScaleFlag.

Referenced by ScalingModel::ScalingModel().
RealMatrix lin_coeffs_modify_n2s (const RealMatrix & src_coeffs, const RealVector & cv_multipliers, const RealVector & lin_multipliers) const [protected]

general linear coefficients mapping from native to scaled space
compute scaled linear constraint matrix given design variable multipliers and linear scaling multipliers. Only scales components corresponding to continuous variables so for src_coeffs of size MxN, lin_multipliers.size() <= M, cv_multipliers.size() <= N
Referenced by ScalingModel::initialize_scaling().

void variables_scaler (const Variables & scaled_vars, Variables & native_vars) [static], [protected]
RecastModel callback for variables scaling: transform variables from scaled to native (user) space.
Variables map from iterator/scaled space to user/native space using a RecastModel.
References Variables::continuous_variable_labels(), Variables::continuous_variables(), ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, ScalingModel::modify_s2n(), Model::outputLevel, and ScalingModel::scaleModelInstance.
Referenced by ScalingModel::ScalingModel().

void secondary_resp_scaler (const Variables & native_vars, const Variables & scaled_vars, const Response & native_response, Response & iterator_response) [static], [protected]
RecastModel callback for secondary response scaling: transform constraints (grads, Hessians) from native (user) to scaled space.
Constraint function map from user/native space to iterator/scaled/combined space using a RecastModel.
References Response::active_set_request_vector(), ScalingModel::need_resp_trans_byvars(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), Model::outputLevel, ScalingModel::response_modify_n2s(), ScalingModel::scaleModelInstance, ScalingModel::secondaryRespScaleFlag, and Response::update_partial.
Referenced by ScalingModel::ScalingModel().

bool need_resp_trans_byvars (const ShortArray & asv, int start_index, int num_resp) const [protected]
determine if response transformation is needed due to variable transformations
Determine if variable transformations present and derivatives requested, which implies a response transformation is necessary
References ScalingModel::varsScaleFlag.
Referenced by ScalingModel::primaryresp_scaler(), ScalingModel::resp_scaled2native(), ScalingModel::secondary_resp_scaled2native(), and ScalingModel::secondaryresp_scaler().

RealVector modify_n2s (const RealVector & native_vars, const IntArray & scale_types, const RealVector & multipliers, const RealVector & offsets) const [protected]

general RealVector mapping from native to scaled variables vectors:
general RealVector mapping from native to scaled variables; loosely, in greatest generality: scaled_var = log((native_var - offset) / multiplier)
Referenced by ScalingModel::initialize_scaling(), and ScalingModel::variables_unscaler().
RealVector modify.s2n ( const RealVector & scaled_vars, const IntArray & scale_types, const RealVector & multipliers, const RealVector & offsets ) const [protected]

general RealVector mapping from scaled to native variables (and values)
  general RealVector mapping from scaled to native variables and/or vals; loosely, in greatest generality: scaled_var = (LOG_BASE^scaled_var) * multiplier + offset

Referenced by ScalingModel::cv_scaled2native(), ScalingModel::secondary_resp.scaled2native(), and ScalingModel::variables_scaler().

void response_modify.n2s ( const Variables & native_vars, const Response & native_response, Response & recast_response, int start_offset, int num_responses ) const [protected]

map responses from native to scaled variable space
  Scaling response mapping: modifies response from a model (user/native) for use in iterators (scaled). Maps num_responses starting at response_offset

References Response::active_set(), Variables::acv(), Variables::all_continuous_variable_ids(), Variables::all_continuous_variables(), Variables::continuous_variable_ids(), Variables::continuous_variables(), Dakota::copy_.data(), Variables::cv(), ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, ActiveSet::derivative_vector(), Dakota::find_index(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian_view(), Response::function_hessians(), Response::function_labels(), Response::function_value(), Response::function_values(), Variables::icv(), Variables::inactive_continuous_variable_ids(), Variables::inactive_continuous_variables(), Model::num_primary_fns(), Model::outputLevel, ActiveSet::request_vector(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, ScalingModel::responseScaleTypes, and Dakota::write_precision.

Referenced by ScalingModel::primary_resp.scaler(), and ScalingModel::secondary_resp.scaler().

void response_modify.s2n ( const Variables & native_vars, const Response & scaled_response, Response & native_response, int start_offset, int num_responses ) const [protected]

map responses from scaled to native space
  Unscaling response mapping: modifies response from scaled (iterator) to native (user) space. Maps num_responses starting at response_offset

References Response::active_set(), Variables::acv(), Variables::all_continuous_variable_ids(), Variables::all_continuous_variables(), Variables::continuous_variable_ids(), Variables::continuous_variables(), Dakota::copy_.data(), Variables::cv(), ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, ActiveSet::derivative_vector(), Dakota::find_index(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian_view(), Response::function_hessians(), Response::function_labels(), Response::function_value(), Response::function_values(), Variables::icv(), Variables::inactive_continuous_variable_ids(), Variables::inactive_continuous_variables(), Model::num_primary_fns(), Model::outputLevel, ActiveSet::request_vector(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, ScalingModel::responseScaleTypes, and Dakota::write_precision.

Referenced by ScalingModel::resp.scaled2native().

13.172.4 Member Data Documentation
ScalningModel * scaleModelInstance [static], [protected]

static pointer to this class for use in static callbacks
  initialization of static needed by RecastModel

  Referenced by ScalingModel::primary_resp.scaler(), ScalingModel::ScalingModel(), ScalingModel::secondary_resp.scaler(), ScalingModel::variables_scaler(), and ScalingModel::variables_unscaler().
13.173 SCALINGOPTIONS CLASS REFERENCE

The documentation for this class was generated from the following files:

- ScalingModel.hpp
- ScalingModel.cpp

13.173 ScalingOptions Class Reference

Simple container for user-provided scaling data, possibly expanded by replicates through the models.

Public Member Functions

- **ScalingOptions ()**
  
  *default ctor: no scaling specified*

- **ScalingOptions (const StringArray &cv_st, RealVector cv_s, const StringArray &pri_st, RealVector pri_s, const StringArray &nln_ineq_st, RealVector nln_ineq_s, const StringArray &nln_eq_st, RealVector nln_eq_s, const StringArray &lin_ineq_st, RealVector lin_ineq_s, const StringArray &lin_eq_st, RealVector lin_eq_s)**

  *standard ctor: scaling from problem DB*

Public Attributes

- **StringArray cvScaleTypes**
- **RealVector cvScales**
- **StringArray priScaleTypes**
- **RealVector priScales**
- **StringArray nlnIneqScaleTypes**
- **RealVector nlnIneqScales**
- **StringArray nlnEqScaleTypes**
- **RealVector nlnEqScales**
- **StringArray linIneqScaleTypes**
- **RealVector linIneqScales**
- **StringArray linEqScaleTypes**
- **RealVector linEqScales**

13.173.1 Detailed Description

Simple container for user-provided scaling data, possibly expanded by replicates through the models.

The documentation for this class was generated from the following file:

- DakotaModel.hpp

13.174 ScilabInterface Class Reference

Inheritance diagram for ScilabInterface:
13.174.1 Detailed Description

Specialization of DirectApplicInterface to link to Scilab analysis drivers. Includes convenience functions to map data to/from Scilab.

The documentation for this class was generated from the following files:

- ScilabInterface.hpp
- ScilabInterface.cpp

13.175 SensAnalysisGlobal Class Reference

Class for a utility class containing correlation calculations and variance-based decomposition.
Public Member Functions

- **SensAnalysisGlobal ()**
  
  *constructor*

- **~SensAnalysisGlobal ()**
  
  *destructor*

- **void compute_correlations (const VariablesArray &vars_samples, const IntResponseMap &resp_samples, const StringSetArray &dss_vals)**
  
  computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank

- **void compute_correlations (const RealMatrix &vars_samples, const IntResponseMap &resp_samples)**
  
  computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank

- **void archive_correlations (const StrStrSizet &run_identifier, ResultsManager &iterator_results, StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView dsv_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels) const**
  
  save correlations to database

- **bool correlations_computed () const**
  
  returns corrComputed to indicate whether compute_correlations() has been invoked

- **void print_correlations (std::ostream &s, StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView dsv_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels) const**
  
  prints the correlations computed in compute_correlations()

Private Member Functions

- **size_t find_valid_samples (const IntResponseMap &resp_samples, BoolDeque &valid_sample)**
  
  find samples with finite response (any sample with any Nan or +/-Inf observation will be dropped)

- **void valid_sample_matrix (const VariablesArray &vars_samples, const IntResponseMap &resp_samples, const StringSetArray &dss_vals, const BoolDeque is_valid_sample, RealMatrix &valid_data)**
  
  extract a compact valid sample (vars/resp) matrix from the passed data

- **void valid_sample_matrix (const RealMatrix &vars_samples, const IntResponseMap &resp_samples, const BoolDeque is_valid_sample, RealMatrix &valid_samples)**
  
  extract a compact valid sample (vars/resp) matrix from the passed data

- **void values_to_ranks (RealMatrix &valid_data)**
  
  replace sample values with their ranks, in-place

- **void center_rows (RealMatrix &data_matrix)**
  
  center the passed matrix by its mean, in-place

- **void correl_adjust (Real &corr_value)**
  
  if result was NaN/Inf, preserve it, otherwise truncate to [-1.0, 1.0]

- **void simple_corr (RealMatrix &total_data, const int &num_in, RealMatrix &corr_matrix)**
  
  computes simple correlations, populating corr_matrix

- **void partial_corr (RealMatrix &total_data, const int num_in, const RealMatrix &simple_corr_mat, RealMatrix &corr_matrix, bool &numerical_issues)**
  
  computes partial correlations, populating corr_matrix and numerical_issues

- **bool has_nan_or_inf (const RealMatrix &corr) const**
  
  Return true if there are any NaN or Inf entries in the matrix.
Static Private Member Functions

- static bool rank_sort (const int &x, const int &y)
  sort algorithm to compute ranks for rank correlations

Private Attributes

- RealMatrix simpleCorr
  matrix to hold simple raw correlations
- RealMatrix simpleRankCorr
  matrix to hold simple rank correlations
- RealMatrix partialCorr
  matrix to hold partial raw correlations
- RealMatrix partialRankCorr
  matrix to hold partial rank correlations
- size_t numFns
  number of responses
- size_t numVars
  number of inputs
- bool numericalIssuesRaw
  flag indicating numerical issues in partial raw correlation calculations
- bool numericalIssuesRank
  flag indicating numerical issues in partial rank correlation calculations
- bool corrComputed
  flag indicating whether correlations have been computed

Static Private Attributes

- static RealArray rawData = RealArray()
  array to hold temporary data before sort

13.175.1 Detailed Description

Class for a utility class containing correlation calculations and variance-based decomposition.

This class provides code for several of the sampling methods both in the NonD branch and in the PStudyD-ACE branch. Currently, the utility functions provide global sensitivity analysis through correlation calculations (e.g. simple, partial, rank, raw) as well as variance-based decomposition.

13.175.2 Member Function Documentation

void compute_correlations ( const VariablesArray & vars_samples, const IntResponseMap & resp_samples, const StringSetArray & dss_vals )

computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank

This version is used when full variables objects are being processed. Calculates simple correlation, partial correlation, simple rank correlation, and partial rank correlation coefficients.
References Dakota::abort_handler(), SensAnalysisGlobal::corrComputed, SensAnalysisGlobal::find_valid_samples(), SensAnalysisGlobal::numericalIssuesRank, SensAnalysisGlobal::numericalIssuesRaw, SensAnalysisGlobal::numFs, SensAnalysisGlobal::numVars, SensAnalysisGlobal::partial_corr(), SensAnalysisGlobal::partialRankCorr, SensAnalysisGlobal::simple_corr(), SensAnalysisGlobal::simpleCorr, SensAnalysisGlobal::simpleRankCorr, SensAnalysisGlobal::valid_sample_matrix(), and SensAnalysisGlobal::values_to_ranks().

Referenced by NonDSampling::compute_statistics(), ParamStudy::post_run(), FSUDesignCompExp::post_run(), and DDACEDesignCompExp::post_run().

```cpp
void compute_correlations ( const RealMatrix & vars_samples, const IntResponseMap & resp_samples )
```

computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank

This version is used when compact samples matrix is being processed. Calculates simple correlation, partial correlation, simple rank correlation, and partial rank correlation coefficients.

References Dakota::abort_handler(), SensAnalysisGlobal::corrComputed, SensAnalysisGlobal::find_valid_samples(), SensAnalysisGlobal::numericalIssuesRank, SensAnalysisGlobal::numericalIssuesRaw, SensAnalysisGlobal::numFs, SensAnalysisGlobal::numVars, SensAnalysisGlobal::partial_corr(), SensAnalysisGlobal::partialRankCorr, SensAnalysisGlobal::simple_corr(), SensAnalysisGlobal::simpleCorr, SensAnalysisGlobal::simpleRankCorr, SensAnalysisGlobal::valid_sample_matrix(), and SensAnalysisGlobal::values_to_ranks().

```cpp
void values_to_ranks ( RealMatrix & valid_data ) [private]
```

replace sample values with their ranks, in-place

When converting values to ranks, uses the average ranks of any tied values

Referenced by SensAnalysisGlobal::compute_correlations().

```cpp
void simple_corr ( RealMatrix & total_data, const int & num_in, RealMatrix & corr_matrix ) [private]
```

computes simple correlations, populating corr_matrix

Calculates simple correlation coefficients from a matrix of data (oriented factors x observations):

- num_corr is number of rows of total data
- num_in indicates whether only pairs of correlations should be calculated between pairs of columns (num_in vs. num_corr-num_in); if num_in = num_corr, correlations are calculated between all columns

References SensAnalysisGlobal::center_rows(), and SensAnalysisGlobal::correl_adjust().

Referenced by SensAnalysisGlobal::compute_correlations().

```cpp
void partial_corr ( RealMatrix & total_data, const int & num_in, const RealMatrix & simple_corr_mat, RealMatrix & corr_matrix, bool & numerical_issues ) [private]
```

computes partial correlations, populating corr_matrix and numerical_issues

Calculates partial correlation coefficients between num_in inputs and numRows() - num_in outputs.

References Dakota::abort_handler(), SensAnalysisGlobal::center_rows(), SensAnalysisGlobal::correl_adjust(), Dakota::qr(), Dakota::qr_rsolve(), and Dakota::svd().

Referenced by SensAnalysisGlobal::compute_correlations().

The documentation for this class was generated from the following files:

- SensAnalysisGlobal.hpp
- SensAnalysisGlobal.cpp
13.176  SeqHybridMetaIterator Class Reference

Method for sequential hybrid iteration using multiple optimization and nonlinear least squares methods on multiple models of varying fidelity.

Inheritance diagram for SeqHybridMetaIterator:

```
            Iterator
              |
              |  
            MetaIterator
              |
                
    SeqHybridMetaIterator
```

Public Member Functions

- `SeqHybridMetaIterator (ProblemDescDB &problem_db)`
  standard constructor
- `SeqHybridMetaIterator (ProblemDescDB &problem_db, Model &model)`
  alternate constructor
- `~SeqHybridMetaIterator ()`
  destructor

Protected Member Functions

- `void core_run ()`
  Performs the hybrid iteration by executing a sequence of iterators, using a similar sequence of models that may vary in fidelity.
- `void print_results (std::ostream &s)`
  print the final iterator results
- `void derived_init_commmunicators (ParLevLIter pl_iter)`
  derived class contributions to initializing the communicators associated with this Iterator instance
- `void derived_set_commmunicators (ParLevLIter pl_iter)`
  derived class contributions to setting the communicators associated with this Iterator instance
- `void derived_free_commmunicators (ParLevLIter pl_iter)`
  derived class contributions to freeing the communicators associated with this Iterator instance
- `IntIntPair estimate_partition_bounds ()`
  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- `const Variables & variables_results () const`
  return the final solution from selectedIterators (variables)
- `const Response & response_results () const`
  return the final solution from selectedIterators (response)
- `void initialize_iterator (int job_index)`
  used by IteratorScheduler to set the starting data for a run
- `void pack_parameters_buffer (MPIPackBuffer &send_buffer, int job_index)`
used by IteratorScheduler to pack starting data for an iterator run

- void unpack_parameters_initialise (MPIUnpackBuffer &recv_buffer, int job_index)

used by IteratorScheduler to unpack starting data and initialize an iterator run

- void pack_results_buffer (MPIPackBuffer &send_buffer, int job_index)

used by IteratorScheduler to pack results data from an iterator run

- void unpack_results_buffer (MPIUnpackBuffer &recv_buffer, int job_index)

used by IteratorScheduler to unpack results data from an iterator run

- void update_local_results (int job_index)

used by IteratorScheduler to update local results arrays

Private Member Functions

- void run_sequential ()
  run a sequential hybrid

- void run_sequential_adaptive ()
  run a sequential adaptive hybrid

- void partition_sets (size_t num_sets, int job_index, size_t &start_index, size_t &job_size)
  convert num_sets and job_index into a start_index and job_size for extraction from parameterSets

- void extract_parameter_sets (int job_index, VariablesArray &partial_param_sets)
  extract partial_param_sets from parameterSets based on job_index

- void update_local_results (PRPArray &prp_results, int job_id)
  update the partial set of final results from the local iterator execution

- void initialize_iterator (const VariablesArray &param_sets)
  called by unpack_parameters_initialise(MPIUnpackBuffer) and initialize_iterator(int) to update the active Model and Iterator

Private Attributes

- String seqHybridType
  empty (default) or "adaptive"

- StringArray methodStrings
  the list of method pointer or method name identifiers

- StringArray modelStrings
  the list of model pointer identifiers for method identification by name

- bool lightwtMethodCtor
  use of lightweight Iterator construction by name

- bool singlePassedModel
  use of constructor that enforces use of a single passed Model

- IteratorArray selectedIterators
  the set of iterators, one for each entry in methodStrings

- ModelArray selectedModels
  the set of models, one for each iterator (if not lightweight construction)

- size_t seqCount
  hybrid sequence counter: 0 to numIterators-1
• Real progressThreshold
going when the progress metric falls below this threshold, the sequential adaptive hybrid switches to the next method

• PRP2DArray prpResults
  2-D array of results corresponding to numIteratorJobs, one set of results per job (iterators may return multiple final solutions)

• VariablesArray parameterSets
  1-D array of variable starting points for the iterator jobs

Friends

• class IteratorScheduler
  protect scheduler callback functions from general access

Additional Inherited Members

13.176.1 Detailed Description

Method for sequential hybrid iteration using multiple optimization and nonlinear least squares methods on multiple models of varying fidelity.

Sequential hybrid meta-iteration supports two approaches: (1) the non-adaptive sequential hybrid runs one method to completion, passes its best results as the starting point for a subsequent method, and continues this succession until all methods have been executed (the stopping rules are controlled internally by each iterator), and (2) the adaptive sequential hybrid uses adaptive stopping rules for the iterators that are controlled externally by this method. Any iterator may be used so long as it defines the notion of a final solution which can be passed as starting data for subsequent iterators.

13.176.2 Member Function Documentation

void print_results ( std::ostream & s ) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Iterator.

References Response::function_values(), Response::is_null(), Variables::is_null(), MetaIterator::iterSched, IteratorScheduler::messagePass, and SeqHybridMetaIterator::prpResults.

void run_sequential ( ) [private]

run a sequential hybrid

In the sequential nonadaptive case, there is no interference with the iterators. Each runs until its own convergence criteria is satisfied. Status: fully operational.

References Iterator::accepts_multiple_points(), ParallelLibrary::bcast(), ParallelLibrary::bcast hs(), Iterator::initialize_graphics(), Model::interface id(), Iterator::iteratedModel, IteratorScheduler::iterator_message_lengths(), IteratorScheduler::iteratorCommRank, IteratorScheduler::iteratorCommSize, IteratorScheduler::iteratorScheduling, IteratorScheduler::iteratorServerId, MetaIterator::iterSched, IteratorScheduler::messagePass, Iterator::methodPCLiter, SeqHybridMetaIterator::methodStrings, IteratorScheduler::miPLIndex, Iterator::num_final_solutions(), IteratorScheduler::numIteratorJobs, IteratorScheduler::numIteratorServers, SeqHybridMetaIterator::pack_parameters_buffer(), Iterator::parallelLib, SeqHybridMetaIterator::parameterSets, SeqHybridMetaIterator::prpResults, ParallelLibrary::recv(), Iterator::response_results(), IteratorScheduler::schedule_iterators(), SeqHybridMetaIterator::selectedIterators,
void run_sequential_adaptive() [private]

run a sequential adaptive hybrid

In the sequential adaptive case, there is interference with the iterators through the use of the ++ overloaded operator. iterator++ runs the iterator for one cycle, after which a progress metric is computed. This progress metric is used to dictate method switching instead of each iterator’s internal convergence criteria. Status: incomplete.

References Iterator::finalize_run(), Iterator::initialize_graphics(), Iterator::initialize_run(), IteratorScheduler::iteratorCommRank, IteratorScheduler::iteratorServerId, MetaIterator::iterSched, SeqHybridMetaIterator::methodStrings, IteratorScheduler::numIteratorServers, SeqHybridMetaIterator::progressThreshold, Iterator::response_results(), SeqHybridMetaIterator::selectedIterators, SeqHybridMetaIterator::selectedModels, SeqHybridMetaIterator::seqCount, Iterator::summaryOutputFlag, and Iterator::variables_results().

Referenced by SeqHybridMetaIterator::core_run().

void extract_parameter_sets(int job_index, VariablesArray & partial_param_sets) [inline], [private]

extract partial_param_sets from parameterSets based on job_index

This convenience function is executed on an iterator master (static scheduling) or a meta-iterator master (self scheduling) at run initialization time and has access to the full parameterSets array (this is All-Reduced for all peers at the completion of each cycle in run_sequential()).

References SeqHybridMetaIterator::parameterSets, and SeqHybridMetaIterator::partition_sets().

Referenced by SeqHybridMetaIterator::initialize_iterators(), and SeqHybridMetaIterator::pack_parameters_buffer().

The documentation for this class was generated from the following files:

- SeqHybridMetaIterator.hpp
- SeqHybridMetaIterator.cpp

### 13.177 SerialDirectApplicInterface Class Reference

Sample derived interface class for testing serial simulator plug-ins using assign_rep().

Inheritance diagram for SerialDirectApplicInterface:
 CHAPTER 13. CLASS DOCUMENTATION

Public Member Functions
• SerialDirectApplicInterface (const Dakota::ProblemDescDB &problem_db)
  constructor
• ~SerialDirectApplicInterface ()
  destructor

Protected Member Functions
• int derived_map_ac (const Dakota::String &ac_name)
  execute an analysis code portion of a direct evaluation invocation
• void derived_map_asynch (const Dakota::ParamResponsePair &pair)
  no-op hides base error; job batching occurs within wait_local_evaluations()
• void wait_local_evaluations (Dakota::PRPQueue &prp_queue)
  evaluate the batch of jobs contained in prp_queue
• void test_local_evaluations (Dakota::PRPQueue &prp_queue)
  invokes wait_local_evaluations() (no special nowait support)
• void set_communicators_checks (int max_eval_concurrency)
  no-op hides default run-time error checks at DirectApplicInterface level

Private Member Functions
• int rosenbrock (const Dakota::RealVector &c_vars, short asv, Dakota::Real &fn_val, Dakota::RealVector &fn_grad, Dakota::RealSymMatrix &fn_hess)
  Rosenbrock plug-in test function.

Additional Inherited Members
13.177.1 Detailed Description
Sample derived interface class for testing serial simulator plug-ins using assign_rep().

The plug-in SerialDirectApplicInterface resides in namespace SIM and uses a copy of rosenbrock() to perform serial parameter to response mappings. It is used to demonstrate plugging in a serial direct analysis driver into Dakota in library mode. Test input files can then use an analysis_driver of "plugin_rosenbrock".

13.177.2 Member Function Documentation
void test_local_evaluations ( Dakota::PRPQueue & prp_queue ) [inline], [protected]
invokes wait_local_evaluations() (no special nowait support)
For use by ApplicationInterface::serve_evaluations_asynch(), which can provide a batch processing capability within message passing schedulers (called using chain IteratorScheduler::run_iterator() -> Model::serve() -> ApplicationInterface::serve_evaluations() -> ApplicationInterface::serve_evaluations_asynch()).
References SerialDirectApplicInterface::wait_local_evaluations().
The documentation for this class was generated from the following files:
• PluginSerialDirectApplicInterface.hpp
• PluginSerialDirectApplicInterface.cpp
13.178  TrackerHTTP::Server Struct Reference

struct to hold tracker/proxy pairs

Public Member Functions

- Server (std::string t, std::string p)

Public Attributes

- std::string tracker
- std::string proxy

13.178.1  Detailed Description

struct to hold tracker/proxy pairs

The documentation for this struct was generated from the following file:

- TrackerHTTP.hpp

13.179  SharedApproxData Class Reference

Base class for the shared approximation data class hierarchy.

Inheritance diagram for SharedApproxData:

```
  SharedApproxData
   `-- SharedPecosApproxData
   `-- SharedSurfpackApproxData
```

Public Member Functions

- SharedApproxData ()  
  default constructor
- SharedApproxData (ProblemDescDB &problem_db, size_t num_vars)  
  standard constructor for envelope
- SharedApproxData (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)  
  alternate constructor for envelope
- SharedApproxData (const SharedApproxData &approx)  
  copy constructor
- virtual ~SharedApproxData ()  
  destructor
- SharedApproxData operator= (const SharedApproxData &approx)  
  assignment operator
- virtual void build ()
builds the shared approximation data from scratch

• virtual void rebuild ()
  rebuilds the shared approximation data incrementally

• virtual void pop (bool save_surr_data)
  back out the previous increment to the shared approximation data

• virtual bool push_available ()
  queries availability of pushing data associated with a trial set

• virtual size_t retrieval_index ()
  return index of trial set within popped bookkeeping sets

• virtual void pre_push ()
  push a previous state of the shared approximation data

• virtual void post_push ()
  clean up popped bookkeeping following push

• virtual size_t finalization_index (size_t i)
  return index of i-th trailing trial set within restorable bookkeeping sets

• virtual void pre_finalize ()
  finalize the shared approximation data following a set of increments

• virtual void post_finalize ()
  clean up popped bookkeeping following aggregation

• virtual void store (size_t index=_NPOS)
  store the current state of the shared approximation data for later combination (defaults to push_back)

• virtual void restore (size_t index=_NPOS)
  restore a previous state of the shared approximation data (defaults to pop_back from stored)

• virtual void remove_stored (size_t index=_NPOS)
  remove an instance of stored approximation data prior to combination (defaults to pop_back)

• virtual size_t pre_combine (short corr_type)
  aggregate the shared approximation data from current and stored states

• virtual void post_combine (short corr_type)
  clean up stored data sets after aggregation

• void set_bounds (const RealVector &c_l_bnds, const RealVector &c_u_bnds, const IntVector &di_l_bnds,
  const IntVector &di_u_bnds, const RealVector &dr_l_bnds, const RealVector &dr_u_bnds)
  set approximation lower and upper bounds (currently only used by graphics)

• SharedApproxData * data_rep () const
  returns dataRep for access to derived class member functions that are not mapped to the top SharedApproxData level

Protected Member Functions

• SharedApproxData (BaseConstructor, ProblemDescDB &problem_db, size_t num_vars)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

• SharedApproxData (NoDBBaseConstructor, const String &approx_type, size_t num_vars, short data_order, short output_level)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
Protected Attributes

- size_t numVars
  number of variables in the approximation
- String approxType
  approximation type identifier
- short buildDataOrder
  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format.
- short outputLevel
  output verbosity level: \{SILENT, QUIET, NORMAL, VERBOSE, DEBUG\} OUTPUT
- String modelExportPrefix
  Prefix for model export files.
- unsigned short modelExportFormat
  Bitmapped format request for exported models.
- RealVector approxCLowerBnds
  approximation continuous lower bounds (used by 3D graphics and Surfpack KrigingModel)
- RealVector approxCUpperBnds
  approximation continuous upper bounds (used by 3D graphics and Surfpack KrigingModel)
- IntVector approxDILowerBnds
  approximation continuous lower bounds
- IntVector approxDIUpperBnds
  approximation continuous upper bounds
- RealVector approxDRLowerBnds
  approximation continuous lower bounds
- RealVector approxDRUpperBnds
  approximation continuous upper bounds

Private Member Functions

- SharedApproxData * get_shared_data (ProblemDescDB &problem_db, size_t num_vars)
  Used only by the standard envelope constructor to initialize dataRep to the appropriate derived type.
- SharedApproxData * get_shared_data (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)
  Used only by the alternate envelope constructor to initialize dataRep to the appropriate derived type.

Private Attributes

- SharedApproxData * dataRep
  pointer to the letter (initialized only for the envelope)
- int referenceCount
  number of objects sharing dataRep
Friends

- class Approximation
- class TaylorApproximation
- class TANA3Approximation
- class GaussProcApproximation
- class VPSApproximation
- class SurfpackApproximation
- class PecosApproximation

13.179.1 Detailed Description

Base class for the shared approximation data class hierarchy.

The SharedApproxData class is the base class for the shared approximation data class hierarchy in DAKOTA. For memory efficiency and enhanced polymorphism, the approximation hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (SharedApproxData) serves as the envelope and one of the derived classes (selected in SharedApproxData::get_shared_data()) serves as the letter.

13.179.2 Constructor & Destructor Documentation

SharedApproxData ( )

default constructor

For the default constructor, dataRep is NULL. This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

Referenced by SharedApproxData::get_shared_data().

SharedApproxData ( ProblemDescDB & problem_db, size_t num_vars )

standard constructor for envelope

Envelope constructor only needs to extract enough data to properly execute get_shared_data, since SharedApproxData(BaseConstructor, problem_db) builds the actual base class data for the derived approximations.

References Dakota::abort_handler(), SharedApproxData::dataRep, and SharedApproxData::get_shared_data().

SharedApproxData ( const String & approx_type, const UShortArray & approx_order, size_t num_vars, short data_order, short output_level )

alternate constructor for envelope

This is the alternate envelope constructor for instantiations on the fly. Since it does not have access to problem_db, it utilizes the NoDBBaseConstructor constructor chain.

References Dakota::abort_handler(), SharedApproxData::dataRep, and SharedApproxData::get_shared_data().

SharedApproxData ( const SharedApproxData & shared_data )

copy constructor

Copy constructor manages sharing of dataRep and incrementing of referenceCount.

References SharedApproxData::dataRep, and SharedApproxData::referenceCount.
SharedApproxData ( ) [virtual]

destructor

Destructor decrements referenceCount and only deletes dataRep when referenceCount reaches zero.
References SharedApproxData::dataRep, and SharedApproxData::referenceCount.

SharedApproxData ( BaseConstructor , ProblemDescDB & problem_db , size_t num_vars ) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_shared_data() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_shared_data() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ~SharedApproxData).
References SharedApproxData::approxType, SharedApproxData::buildDataOrder, ProblemDescDB::get_bool(), ProblemDescDB::get_db_model_node(), ProblemDescDB::get_string(), ProblemDescDB::set_db_model_nodes(), Dakota::strbegins(), and Dakota::strends().

SharedApproxData ( NoDBBaseConstructor , const String & approx_type , size_t num_vars , short data_order , short output_level ) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_shared_data() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_shared_data() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ~SharedApproxData).
References SharedApproxData::approxType, SharedApproxData::buildDataOrder, Dakota::strbegins(), and Dakota::strends().

13.179.3 Member Function Documentation

SharedApproxData operator= ( const SharedApproxData & shared_data )

assignment operator

References SharedApproxData::dataRep, and SharedApproxData::referenceCount.

SharedApproxData * get_shared_data ( ProblemDescDB & problem_db , size_t num_vars ) [private]

Used only by the standard envelope constructor to initialize dataRep to the appropriate derived type.

Used only by the envelope constructor to initialize dataRep to the appropriate derived type.
References ProblemDescDB::get_string(), SharedApproxData::SharedApproxData(), and Dakota::strends().
Referenced by SharedApproxData::SharedApproxData().

SharedApproxData * get_shared_data ( const String & approx_type , const UShortArray & approx_order , size_t num_vars , short data_order , short output_level ) [private]

Used only by the alternate envelope constructor to initialize dataRep to the appropriate derived type.
13.179.4 Member Data Documentation

**short buildDataOrder [protected]**  
order of the data used for surrogate construction, in *Active* request vector 3-bit format.

This setting distinguishes derivative data intended for use in construction (includes derivatives w.r.t. the build variables) from derivative data that may be approximated separately (excludes derivatives w.r.t. auxilliary variables). This setting should also not be inferred directly from the responses specification, since we may need gradient support for evaluating gradients at a single point (e.g., the center of a trust region), but not require gradient evaluations at every point.

Referenced by SharedSurfpackApproxData::add_sd_to_surfdata(), TaylorApproximation::build(), TaylorApproximation::gradient(), TaylorApproximation::hessian(), TaylorApproximation::min_coefficients(), Approximation::min_points(), Approximation::recommended_points(), SharedApproxData::SharedApproxData(), SharedPecosApproxData::SharedPecosApproxData(), SurfpackApproximation::SurfpackApproximation(), SurfpackApproximation::surrogates_to_surfdata(), TANA3Approximation::TANA3Approximation(), and TaylorApproximation::value().

The documentation for this class was generated from the following files:

- SharedApproxData.hpp
- SharedApproxData.cpp

13.180 SharedPecosApproxData Class Reference

Derived approximation class for global basis polynomials.

Inheritance diagram for SharedPecosApproxData:

```
SharedApproxData
  SharedPecosApproxData
```

**Public Member Functions**

- **SharedPecosApproxData ()**  
  default constructor  

- **SharedPecosApproxData (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)**  
  alternate constructor  

- **SharedPecosApproxData (ProblemDescDB &problem_db, size_t num_vars)**  
  standard ProblemDescDB-driven constructor  

- **~SharedPecosApproxData ()**  
  destructor  

- **void random_variables_key (const Pecos::BitArray &random_vars_key)**  
  set pecosBasisApprox.randomVarsKey
void integration_iterator (const Iterator &iterator)
  set pecosBasisApprox.driverRep
• void construct_basis (const Pecos::ShortArray &u_types, const Pecos::AleatoryDistParams &adp)
  invoke Pecos::SharedOrthogPolyApproxData::construct_basis()
• void polynomial_basis (const std::vector<Pecos::BasisPolynomial> &poly_basis)
  set Pecos::SharedOrthogPolyApproxData::polynomialBasis
• const std::vector<Pecos::BasisPolynomial> & polynomial_basis () const
  get Pecos::SharedOrthogPolyApproxData::polynomialBasis
• std::vector<Pecos::BasisPolynomial> & polynomial_basis ()
  get Pecos::SharedOrthogPolyApproxData::polynomialBasis
• void allocate (const UShort2DArray &mi)
  set Pecos::SharedOrthogPolyApproxData::multiIndex and allocate associated arrays
• const UShort2DArray & multi_index () const
  get Pecos::SharedOrthogPolyApproxData::multiIndex
• const Pecos::BitArrayULongMap & sobol_index_map () const
  return Pecos::SharedPolyApproxData::sobolIndexMap
• void coefficients_norms_flag (bool flag)
  invoke Pecos::SharedOrthogPolyApproxData::coefficients_norms_flag()
• size_t expansion_terms () const
  return Pecos::SharedOrthogPolyApproxData::expansion_terms()
• const UShortArray & expansion_order () const
  return Pecos::SharedOrthogPolyApproxData::expansion_order()
• void expansion_order (const UShortArray &order)
  invokes Pecos::SharedOrthogPolyApproxData::expansion_order(UShortArray&)
• void increment_order ()
  invokes Pecos::SharedOrthogPolyApproxData::increment_order()
• void configuration_options (const Pecos::ExpansionConfigOptions &ec_options)
  set the expansion configuration options within Pecos::SharedPolyApproxData
• void configuration_options (const Pecos::BasisConfigOptions &bc_options)
  set the basis configuration options within Pecos::SharedPolyApproxData
• void configuration_options (const Pecos::RegressionConfigOptions &rc_options)
  set the regression configuration options within Pecos::SharedRegressOrthogPolyApproxData

Protected Member Functions

• void build ()
  builds the shared approximation data from scratch
• void rebuild ()
  rebuilds the shared approximation data incrementally
• void pop (bool save_surr_data)
  back out the previous increment to the shared approximation data
• bool push_available ()
queries availability of pushing data associated with a trial set

- `size_t retrieval_index()`
  return index of trial set within popped bookkeeping sets

- `void pre_push()`
  push a previous state of the shared approximation data

- `void post_push()`
  clean up popped bookkeeping following push

- `size_t finalization_index(size_t i)`
  return index of i-th trailing trial set within restorable bookkeeping sets

- `void pre_finalize()`
  finalize the shared approximation data following a set of increments

- `void post_finalize()`
  clean up popped bookkeeping following aggregation

- `void store(size_t index=_NPOS)`
  store the current state of the shared approximation data for later combination (defaults to push_back)

- `void restore(size_t index=_NPOS)`
  restore a previous state of the shared approximation data (defaults to pop_back from stored)

- `void remove_stored(size_t index=_NPOS)`
  remove an instance of stored approximation data prior to combination (defaults to pop_back)

- `size_t pre_combine(short corr_type)`
  aggregate the shared approximation data from current and stored states

- `void post_combine(short corr_type)`
  clean up stored data sets after aggregation

### Private Member Functions

- `Pecos::SharedBasisApproxData & pecos_shared_data()`
  return pecosSharedData

- `void approx_type_to_basis_type(const String &approx_type, short &basis_type)`
  utility to convert Dakota type string to Pecos type enumeration

### Private Attributes

- `Pecos::SharedBasisApproxData pecosSharedData`
  the Pecos shared approximation data

- `Pecos::SharedPolyApproxData * pecosSharedDataRep`
  convenience pointer to derived letter within pecosSharedData

### Friends

- `class PecosApproximation`
13.180.1 Detailed Description

Derived approximation class for global basis polynomials.

The SharedPecosApproxData class provides a global approximation based on basis polynomials. This includes orthogonal polynomials used for polynomial chaos expansions and interpolation polynomials used for stochastic collocation.

The documentation for this class was generated from the following files:

- SharedPecosApproxData.hpp
- SharedPecosApproxData.cpp

13.181 SharedResponseData Class Reference

Container class encapsulating variables data that can be shared among a set of Response instances.

Public Member Functions

- SharedResponseData ()
  default constructor
- SharedResponseData (const ProblemDescDB &problem_db)
  standard constructor
- SharedResponseData (const ActiveSet &set)
  alternate on-the-fly constructor (explicit disallows its use for implicit type conversion so that instantiations of Response(set) are invalid)
- SharedResponseData (const SharedResponseData &srd)
  copy constructor
- ~SharedResponseData ()
  destructor
- SharedResponseData & operator= (const SharedResponseData &srd)
  assignment operator
- bool operator== (const SharedResponseData &other)
  experimental operator== for use in unit testing
- size_t num_scalar_responses () const
  number of scalar responses
- size_t num_field_response_groups () const
  number of field response groups
- size_t num_response_groups () const
  total number of response groups (scalars + field groups)
- size_t num_field_functions () const
  total number of field functions (1-norm of fieldRespGroupLengths)
- size_t num_functions () const
  total number of response functions (scalars + 1-norm of fieldRespGroupLengths)
- const IntVector & field_lengths () const
  index of field lengths for field data
void field_lengths (const IntVector &field_lengths)
    set field lengths (if experiment different from simulation)
const IntVector & num_coords_per_field () const
    dimensions of each function
const String & function_label (size_t i) const
    return a response function identifier string
const StringArray & function_labels () const
    return the response function identifier strings
StringArray & function_labels ()
    return the response function identifier strings
void function_label (const String &label, size_t i)
    set a response function identifier string
void function_labels (const StringArray &labels)
    set the response function identifier strings
const StringArray & field_group_labels ()
    return the coarse (per-group) field response labels
void field_group_labels (const StringArray &field_labels)
    set the coarse field group labels (must agree with number fields)
const String & responses_id () const
    return the response identifier
short response_type () const
    return the response type: {BASE, SIMULATION, EXPERIMENT}.RESPONSE
void response_type (short type)
    set the response type: {BASE, SIMULATION, EXPERIMENT}.RESPONSE
short primary_fn_type () const
    get the primary function type (generic, objective, calibration)
void primary_fn_type (short type)
    set the primary function type (generic, objective, calibration)
SharedResponseData copy () const
    create a deep copy of the current object and return by value
void reshape (size_t num_fns)
    reshape the data, disconnecting a shared rep if necessary
bool is_null () const
    return true if empty handle with null representation
long reference_count () const
    how many handles (including this) are sharing this representation (body); for debugging/testing only
template<class Archive>
void serialize (Archive &ar, const unsigned int version)
    serialize through the pointer, which requires object tracking; write and read are symmetric for this class

Private Member Functions


Private Attributes

- boost::shared_ptr
  \< SharedResponseDataRep \> srdRep
  pointer to the body (handle-body idiom)

Friends

- class boost::serialization::access
  allow boost access to serialize this class

13.181.1 Detailed Description

Container class encapsulating variables data that can be shared among a set of Response instances.

An array of Response objects (e.g., Analyzer::allResponse) contains repeated configuration data (id’s, labels, counts), SharedResponseData employs a handle-body idiom to allow this shared data to be managed in a single object with many references to it, one per Response object in the array. This allows scaling to larger sample sets.

13.181.2 Member Function Documentation

SharedResponseData copy ( ) const
create a deep copy of the current object and return by value
Deep copies are used when recasting changes the nature of a Response set.
References SharedResponseData::srdRep.
Referenced by ExperimentData::initialize(), and ExperimentData::load_data().
The documentation for this class was generated from the following files:

- SharedResponseData.hpp
- SharedResponseData.cpp

13.182 SharedResponseDataRep Class Reference

The representation of a SharedResponseData instance. This representation, or body, may be shared by multiple SharedResponseData handle instances.

Public Member Functions

- ~SharedResponseDataRep ()
  destructor must be public for shared_ptr
- template<class Archive >
  void serialize (Archive &ar, const unsigned int version)

Private Member Functions

- SharedResponseDataRep ()
  default constructor
- SharedResponseDataRep (const ProblemDescDB &problem_db)
  standard constructor
CHAPTER 13. CLASS DOCUMENTATION

- **SharedResponseDataRep** (const `ActiveSet` &set)
  alternate on-the-fly constructor
- **void copy_rep** (SharedResponseDataRep *srd_rep)
  copy the data from srd_rep to the current representation
- **template<class Archive>**
  void **serialize** (Archive &ar, const unsigned int version)
  serialize the core shared response data: write and read are symmetric for this class
- **bool operator==** (const SharedResponseDataRep &other)
  experimental operator== for use in unit testing
- **void build_field_labels ()**
  build/update the unrolled field labels based on fieldLabels and group lengths

**Private Attributes**

- **short responseType**
  enumeration of BASE_RESPONSE, SIMULATION_RESPONSE, or EXPERIMENT_RESPONSE
- **short primaryFnType**
  data set type for primary response: generic, objective, calibration
- **String responsesId**
  response identifier string from the input file
- **StringArray functionLabels**
  fine-grained (unrolled) set of response function identifiers used to improve output readability; length Response-::functionValues
- **StringArray fieldLabels**
  labels for each field group
- **size_t numScalarResponses**
  number of scalar responses
- **IntVector fieldRespGroupLengths**
  index of field lengths for field data
- **IntVector numCoordsPerField**
  dimensions of each function

**Friends**

- **class SharedResponseData**
- **class boost::serialization::access**
  allow boost access to serialize this class

**13.182.1 Detailed Description**

The representation of a **SharedResponseData** instance. This representation, or body, may be shared by multiple **SharedResponseData** handle instances.

The SharedResponseData/SharedResponseDataRep pairs utilize a handle-body idiom (Coplien, Advanced C++).
### 13.182.2 Member Function Documentation

```cpp
void copy_rep ( SharedResponseDataRep * srd_rep ) [private]
```

copy the data from srd_rep to the current representation

Deep copies are used when recasting changes the nature of a `Response` set.

References `SharedResponseDataRep::fieldLabels`, `SharedResponseDataRep::fieldRespGroupLengths`, `SharedResponseDataRep::functionLabels`, `SharedResponseDataRep::numCoordsPerField`, `SharedResponseDataRep::numScalarResponses`, `SharedResponseDataRep::primaryFnType`, `SharedResponseDataRep::responsesId`, and `SharedResponseDataRep::responseType`.

The documentation for this class was generated from the following files:

- `SharedResponseData.hpp`
- `SharedResponseData.cpp`

### 13.183 SharedSurfpackApproxData Class Reference

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

Inheritance diagram for `SharedSurfpackApproxData`:

```
SharedApproxData
  SharedSurfpackApproxData
```

#### Public Member Functions

- `SharedSurfpackApproxData ()`
  *default constructor*

- `SharedSurfpackApproxData (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)`
  *alternate constructor*

- `SharedSurfpackApproxData (ProblemDescDB &problem_db, size_t num_vars)`
  *standard constructor: Surfpack surface of appropriate type will be created*

- `~SharedSurfpackApproxData ()`
  *destructor*

#### Private Member Functions

- `void add_sd_to_surfdata (const Pecos::SurrogateDataVars &sdv, const Pecos::SurrogateDataResp &sdr, short fail_code, SurfData &surf_data)`
  *add Pecos::SurrogateData{Vars,Resp} to SurfData, accounting for buildDataOrder available*

- `void copy_matrix (const RealSymMatrix &rsm, SurfpackMatrix< Real > &surfpack_matrix)`
  *copy RealSymMatrix to SurfpackMatrix (Real type only)*

- `void merge_variable_arrays (const RealVector &cv, const IntVector &div, const RealVector &drv, RealArray &ra)`

---

13.183. SHARESURFPACKAPPROXDATA CLASS REFERENCE
merge cv, div, and drv vectors into a single ra array

- void sdv_to_realarray (const Pecos::SurrogateDataVars &sdv, RealArray &ra)
  aggregate \{ continuous, discrete int, discrete real \} variables from SurrogateDataVars into ra

- void vars_to_realarray (const Variables &vars, RealArray &ra)
  aggregate \{ active, all \} \{ continuous, discrete int, discrete real \} variables into ra

Private Attributes

- unsigned short approxOrder
  order of polynomial approximation

- StringArray diagnosticSet
  set of diagnostic metrics

- bool crossValidateFlag
  whether to perform cross validation

- unsigned numFolds
  number of folds for CV

- Real percentFold
  percentage of data for CV

- bool pressFlag
  whether to perform PRESS

Friends

- class SurfpackApproximation
- class VPSApproximation

Additional Inherited Members

13.183.1 Detailed Description

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

The SharedSurfpackApproxData class is the interface between Dakota and Surfpack. Based on the information in the ProblemDescDB that is passed in through the constructor, SharedSurfpackApproxData builds a Surfpack Surface object that corresponds to one of the following data-fitting techniques: polynomial regression, kriging, artificial neural networks, radial basis function network, or multivariate adaptive regression splines (MARS).

13.183.2 Constructor & Destructor Documentation

SharedSurfpackApproxData ( const String & approx_type, const UShortArray & approx_order, size_t num_vars, short data_order, short output_level )

alternate constructor
  On-the-fly constructor which uses mostly Surfpack model defaults.

  References Dakota::abort_handler(), SharedSurfpackApproxData::approxOrder, and SharedApproxData::approxType.
SharedSurfpackApproxData ( ProblemDescDB & problem_db, size_t num_vars )

standard constructor: Surfpack surface of appropriate type will be created
  Initialize the embedded Surfpack surface object and configure it using the specifications from the input file.
  Data for the surface is created later.
  References SharedSurfpackApproxData::approxOrder, SharedApproxData::approxType, ProblemDescDB::get_short(), and ProblemDescDB::get_string().
  The documentation for this class was generated from the following files:

  • SharedSurfpackApproxData.hpp
  • SharedSurfpackApproxData.cpp

13.184 SharedVariablesData Class Reference

Container class encapsulating variables data that can be shared among a set of Variables instances.

Public Member Functions

  • SharedVariablesData ()
    default constructor
  • SharedVariablesData (const ProblemDescDB &problem_db, const std::pair< short, short >& view)
    standard constructor
  • SharedVariablesData (const std::pair< short, short >& view, const std::map< unsigned short, size_t >& vars_comps, const BitArray & all_relax_di=BitArray(), const BitArray & all_relax_dr=BitArray())
    medium weight constructor providing detailed variable counts
  • SharedVariablesData (const std::pair< short, short >& view, const SizetArray & vars_comps_totals, const BitArray & all_relax_di=BitArray(), const BitArray & all_relax_dr=BitArray())
    lightweight constructor providing variable count totals
  • SharedVariablesData (const SharedVariablesData & svd)
    copy constructor
  • ~SharedVariablesData ()
    destructor
  • SharedVariablesData & operator= (const SharedVariablesData & svd)
    assignment operator
  • SharedVariablesData copy () const
    create a deep copy of the current object and return by value
  • void all_counts (size_t & num_acv, size_t & num_adiv, size_t & num_adsv, size_t & num_adrv) const
    compute all variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete(Int,Real)
  • void design_counts (size_t & num_cdv, size_t & num_ddiv, size_t & num_ddsv, size_t & num_ddrv) const
    compute design variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete(Int,Real)
  • void aleatory_uncertain_counts (size_t & num_cauv, size_t & num dauiv, size_t & num_dausv, size_t & num_daurv) const
    compute aleatory uncertain variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete(Int,Real)
• void epistemic_uncertain_counts (size_t &num_ceuv, size_t &num_deuiv, size_t &num_deusv, size_t &num_deurv) const
  compute epistemic uncertain variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete[Int,Real]
• void uncertain_counts (size_t &num_cuv, size_t &num_duiv, size_t &num_dusv, size_t &num_durv) const
  compute uncertain variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete[Int,Real]
• void state_counts (size_t &num_csv, size_t &num_dsiv, size_t &num_dssv, size_t &num_dsrv) const
  compute state variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete[Int,Real]
• void initialize_active_start_counts ()
  initialize start index and counts for active variables
• void initialize_inactive_start_counts ()
  initialize start index and counts for inactive variables
• void initialize_active_components ()
  initialize the active components totals given active variable counts
• void initialize_inactive_components ()
  initialize the inactive components totals given inactive variable counts
• const BitArray & all_relaxed_discrete_int () const
  return allRelaxedDiscreteInt
• const BitArray & all_relaxed_discrete_real () const
  return allRelaxedDiscreteReal
• StringMultiArrayView all_continuous_labels (size_t start, size_t num_items) const
  get num_items continuous labels beginning at index start
• void all_continuous_labels (StringMultiArrayConstView cv_labels, size_t start, size_t num_items)
  set num_items continuous labels beginning at index start
• void all_continuous_label (const String &cv_label, size_t index)
  set continuous label at index start
• StringMultiArrayView all_discrete_int_labels (size_t start, size_t num_items) const
  get num_items discrete integer labels beginning at index start
• void all_discrete_int_labels (StringMultiArrayConstView div_labels, size_t start, size_t num_items)
  set num_items discrete integer labels beginning at index start
• void all_discrete_int_label (const String &div_label, size_t index)
  set discrete integer label at index start
• StringMultiArrayView all_discrete_string_labels (size_t start, size_t num_items) const
  get num_items discrete string labels beginning at index start
• void all_discrete_string_labels (StringMultiArrayConstView dsv_labels, size_t start, size_t num_items)
  set num_items discrete string labels beginning at index start
• void all_discrete_string_label (const String &dsv_label, size_t index)
  set discrete string label at index start
• StringMultiArrayView all_discrete_real_labels (size_t start, size_t num_items) const
  get num_items discrete real labels beginning at index start
• void all_discrete_real_labels (StringMultiArrayConstView drv_labels, size_t start, size_t num_items)
  set num_items discrete real labels beginning at index start
void all_discrete_real_label (const String &drv_label, size_t index)  
set discrete real label at index start

UShortMultiArrayConstView all_continuous_types (size_t start, size_t num_items) const
get num_items continuous types beginning at index start

void all_continuous_types (UShortMultiArrayConstView cv_types, size_t start, size_t num_items)
set num_items continuous types beginning at index start

void all_continuous_type (unsigned short cv_type, size_t index)
set continuous type at index

UShortMultiArrayConstView all_discrete_int_types (size_t start, size_t num_items) const
get num_items discrete integer types beginning at index start

void all_discrete_int_types (UShortMultiArrayConstView div_types, size_t start, size_t num_items)
set num_items discrete integer types beginning at index start

void all_discrete_int_type (unsigned short div_type, size_t index)
set discrete integer type at index

UShortMultiArrayConstView all_discrete_string_types (size_t start, size_t num_items) const
get num_items discrete string types beginning at index start

void all_discrete_string_types (UShortMultiArrayConstView dsv_types, size_t start, size_t num_items)
set num_items discrete string types beginning at index start

void all_discrete_string_type (unsigned short dsv_type, size_t index)
set discrete string type at index

UShortMultiArrayConstView all_discrete_real_types (size_t start, size_t num_items) const
get num_items discrete real types beginning at index start

void all_discrete_real_types (UShortMultiArrayConstView drv_types, size_t start, size_t num_items)
set num_items discrete real types beginning at index start

void all_discrete_real_type (unsigned short drv_type, size_t index)
set discrete real type at index

SizetMultiArrayConstView all_continuous_ids (size_t start, size_t num_items) const
get num_items continuous ids beginning at index start

void all_continuous_ids (SizetMultiArrayConstView cv_ids, size_t start, size_t num_items)
set num_items continuous ids beginning at index start

void all_continuous_id (size_t id, size_t index)
set num_items continuous ids beginning at index start

const String & id () const
return the user-provided or default Variables identifier

const SizetArray & components_totals () const
return variable type counts for \{continuous,discrete integer,discrete real\} \{design,aleatory uncertain,epistemic uncertain,state\}

const SizetArray & active_components_totals () const
return active variable type counts for \{continuous,discrete integer,discrete real\} \{design,aleatory uncertain,epistemic uncertain,state\}

const SizetArray & inactive_components_totals () const
return inactive variable type counts for \{continuous,discrete integer,discrete real\} \{design,aleatory uncertain,epistemic uncertain,state\}

size_t vc_lookup (unsigned short key) const
retrieve the variables type count within svdRep->variablesComponents corresponding to (a fine-grain variables type) key

- const std::pair< short, short > & view () const
  retrieve the Variables view

- void inactive_view (short view2)
  set the inactive Variables view

- size_t cv () const
  get number of active continuous vars

- size_t cv_start () const
  get start index of active continuous vars

- size_t div () const
  get number of active discrete int vars

- size_t div_start () const
  get start index of active discrete int vars

- size_t dsv () const
  get number of active discrete string vars

- size_t dsv_start () const
  get start index of active discrete string vars

- size_t drv () const
  get number of active discrete real vars

- size_t drv_start () const
  get start index of active discrete real vars

- size_t icv () const
  get number of inactive continuous vars

- size_t icv_start () const
  get start index of inactive continuous vars

- size_t idiv () const
  get number of inactive discrete int vars

- size_t idiv_start () const
  get start index of inactive discrete int vars

- size_t idsv () const
  get number of inactive discrete string vars

- size_t idsv_start () const
  get start index of inactive discrete string vars

- size_t idrv () const
  get number of inactive discrete real vars

- size_t idrv_start () const
  get start index of inactive discrete real vars

- void cv (size_t ncv)
  set number of active continuous vars

- void cv_start (size_t cvs)
  set start index of active continuous vars

- void div (size_t ndiv)
set number of active discrete int vars
• void div_start(size_t divs)
set start index of active discrete int vars
• void dsv (size_t ndsv)
set number of active discrete string vars
• void dsv_start (size_t dsvs)
set start index of active discr string vars
• void drv (size_t ndrv)
set number of active discrete real vars
• void drv_start (size_t drvs)
set start index of active discrete real vars
• void icv (size_t nicv)
set number of inactive continuous vars
• void icv_start (size_t icvs)
set start index of inactive continuous vars
• void idiv (size_t nidiv)
set number of inactive discrete int vars
• void idiv_start (size_t idivs)
set start index of inactive discr int vars
• void idsv (size_t nidsv)
set number of inactive discr string vars
• void idsv_start (size_t idsvs)
set start index of inact discr string vars
• void idrv (size_t nidrv)
set number of inactive discrete real vars
• void idrv_start (size_t idrvs)
set start index of inact discr real vars
• template<class Archive>
void serialize (Archive &ar, const unsigned int version)

Private Member Functions
• template<class Archive>
void serialize (Archive &ar, const unsigned int version)

serialize through the pointer, which requires object tracking: write and read are symmetric for this class

Private Attributes
• boost::shared_ptr
< SharedVariablesDataRep > svdRep
pointer to the body (handle-body idiom)

Friends
• class boost::serialization::access
allow boost access to serialize this class
13.184.1 Detailed Description

Container class encapsulating variables data that can be shared among a set of Variables instances.

An array of Variables objects (e.g., Analyzer::allVariables) contains repeated configuration data (id’s, labels, counts). SharedVariablesData employs a handle-body idiom to allow this shared data to be managed in a single object with many references to it, one per Variables object in the array. This allows scaling to larger sample sets.

13.184.2 Member Function Documentation

SharedVariablesData copy ( ) const

create a deep copy of the current object and return by value

Deep copies are used when recasting changes the nature of a Variables set. References Dakota::svd(), and SharedVariablesData::svdRep.

The documentation for this class was generated from the following files:

- SharedVariablesData.hpp
- SharedVariablesData.cpp

13.185 SharedVariablesDataRep Class Reference

The representation of a SharedVariablesData instance. This representation, or body, may be shared by multiple SharedVariablesData handle instances.

Public Member Functions

- ~SharedVariablesDataRep ()
  destructor must be public for shared_ptr
- template<class Archive>
  void save (Archive &ar, const unsigned int version) const
- template<class Archive>
  void load (Archive &ar, const unsigned int version)

Private Member Functions

- SharedVariablesDataRep (const ProblemDescDB &problem db, const std::pair< short, short > &view)
  standard constructor
- SharedVariablesDataRep (const std::pair< short, short > &view, const std::map< unsigned short, size_t > &vars_comps, const BitArray &all_relax_di, const BitArray &all_relax_dr)
  medium weight constructor providing detailed variable counts
- SharedVariablesDataRep (const std::pair< short, short > &view, const SizetArray &vars_comps_totals, const BitArray &all_relax_di, const BitArray &all_relax_dr)
  lightweight constructor providing variable count totals
- SharedVariablesDataRep ()
  default constructor
- void initialize_components_totals (const ProblemDescDB &problem_db)
  populate variables{Components,CompsTotals} from user variable type and count specifications
- void components_to_totals ()
update variablesCompsTotals from variablesComponents

- **void relax_noncategorical** (const ProblemDescDB &problem_db)
  populate allRelaxedDiscrete{Int,Real} from user specifications (relax variables that are not declared as categorical)

- **void set_relax** (const BitArray &user_cat_spec, size_t ucs_index, size_t ard_cntr, BitArray &ard_container)
  Set the ard_cntr entry in the all-relaxed-discrete integer or real container ard_container, based on user-specification of categorical, accounting for empty.

- **void all_counts** (size_t &num_acv, size_t &num_adiv, size_t &num_adsv, size_t &num_adrv) const
  compute all variables sums from variablesCompsTotals

- **void relax_counts** (size_t &num_cv, size_t &num_div, size_t &num_dr, size_t offset_di, size_t offset_dr) const
  adjust counts based on allRelaxedDiscrete{Int,Real}

- **void design_counts** (size_t &num_cdv, size_t &num_ddiv, size_t &num_ddsv, size_t &num_ddrv) const
  compute design variables sums from variablesCompsTotals

- **void aleatory_uncertain_counts** (size_t &num_cauv, size_t &num_dauiv, size_t &num_dausv, size_t &num_dauurv) const
  compute aleatory uncertain variables sums from variablesCompsTotals

- **void epistemic_uncertain_counts** (size_t &num_ceuv, size_t &num_deuiv, size_t &num_deusv, size_t &num_deurv) const
  compute epistemic uncertain variables sums from variablesCompsTotals

- **void uncertain_counts** (size_t &num_cuv, size_t &num_dauv, size_t &num_dusv, size_t &num_durv) const
  compute uncertain variables sums from variablesCompsTotals

- **void state_counts** (size_t &num_csv, size_t &num_dsv, size_t &num_dsv, size_t &num_dsvr) const
  compute state variables sums from variablesCompsTotals

- **void view_start_counts** (short view, size_t &cv_start, size_t &div_start, size_t &dsv_start, size_t &drv_start, size_t &num_cv, size_t &num_div, size_t &num_dsv, size_t &num_drv) const
  define start indices and counts for active variables based on view

- **void size_all_labels** ()
  size all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Labels, with or without discrete relaxation

- **void size_all_types** ()
  size all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Types, with or without discrete relaxation

- **void initialize_all_labels** (const ProblemDescDB &problem_db)
  aggregate all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Labels from user specification or defaults

- **void initialize_all_types** ()
  initialize all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Types, with or without discrete relaxation

- **void initialize_all_jds** ()
  initialize allContinuousIds (discrete not currently needed), with or without discrete relaxation

- **void initialize_active_start_counts** ()
  initialize {c,di,dr}\Start and num{D,DI,DS,DR}V

- **void initialize_inactive_start_counts** ()
  initialize i{c,di,dr}\Start and numl{D,DI,DS,DR}V

- **void initialize_active_components** ()
  initialize activeVarsCompsTotals given {c,di,dr}v\Start and numl{C,DI,DR}V

- **void initialize_inactive_components** ()
initialize inactiveVarsCompsTotals given \{c,di,dr\}vStart and numI\{C,DI,DR\}V

- size_t vc_lookup (unsigned short key) const
  retrieve the count within variablesComponents corresponding to key

- void copy_rep (SharedVariablesDataRep *svd_rep)
  copy the data from svd_rep to the current representation

- template<class Archive>
  void save (Archive &ar, const unsigned int version) const
  serialize the core shared variables data

- template<class Archive>
  void load (Archive &ar, const unsigned int version)
  load the core shared variables data and restore class state

- BOOST_SERIALIZATION_SPLIT_MEMBER () String variablesId
  variables identifier string from the input file

Private Attributes

- std::map< unsigned short, size_t > variablesComponents
  map linking variable types to counts

- SizetArray variablesCompsTotals
  totals for variable type counts for \{\text{continuous,discrete integer,discrete string,discrete real}\} \{\text{design,aleatory uncertain,epistemic uncertain,state}\}.

- SizetArray activeVarsCompsTotals
  totals for active variable type counts for \{\text{continuous,discrete integer,discrete string,discrete real}\} \{\text{design,aleatory uncertain,epistemic uncertain,state}\}.

- SizetArray inactiveVarsCompsTotals
  totals for inactive variable type counts for \{\text{continuous,discrete integer,discrete string,discrete real}\} \{\text{design,aleatory uncertain,epistemic uncertain,state}\}.

- std::pair< short, short > variablesView
  the variables view pair containing active (first) and inactive (second) view enumerations

- size_t cvStart
  start index of active continuous variables within allContinuousVars

- size_t divStart
  start index of active discrete integer variables within allDiscreteIntVars

- size_t dsvStart
  start index of active discrete string vars within allDiscreteStringVars

- size_t drvStart
  start index of active discrete real variables within allDiscreteRealVars

- size_t icvStart
  start index of inactive continuous variables within allContinuousVars

- size_t idivStart
  start index of inactive discrete integer vars within allDiscreteIntVars

- size_t idsvStart
  start index of inactive discrete string vars within allDiscreteStringVars

- size_t idrvStart
13.185. SHAREDVARIABLESDATAREP CLASS REFERENCE

start index of inactive discrete real variables within allDiscreteRealVars

- size_t numCV
  number of active continuous variables
- size_t numDIV
  number of active discrete integer variables
- size_t numDSV
  number of active discrete string variables
- size_t numDRV
  number of active discrete real variables
- size_t numICV
  number of inactive continuous variables
- size_t numIDIV
  number of inactive discrete integer variables
- size_t numIDSV
  number of inactive discrete string variables
- size_t numIDRV
  number of inactive discrete real variables

- StringMultiArray allContinuousLabels
  array of variable labels for all of the continuous variables
- StringMultiArray allDiscreteIntLabels
  array of variable labels for all of the discrete integer variables
- StringMultiArray allDiscreteStringLabels
  array of variable labels for all of the discrete string variables
- StringMultiArray allDiscreteRealLabels
  array of variable labels for all of the discrete real variables
- UShortMultiArray allContinuousTypes
  array of variable types for all of the continuous variables
- UShortMultiArray allDiscreteIntTypes
  array of variable types for all of the discrete integer variables
- UShortMultiArray allDiscreteStringTypes
  array of variable types for all of the discrete string variables
- UShortMultiArray allDiscreteRealTypes
  array of variable types for all of the discrete real variables
- SizetMultiArray allContinuousIds
  array of 1-based position identifiers for the all continuous variables array
- BitArray allRelaxedDiscreteInt
  array of booleans to indicate relaxation (promotion from DiscreteInt to Continuous) for all specified discrete int variables Note: container will be empty when not relaxing variables
- BitArray allRelaxedDiscreteReal
  array of booleans to indicate relaxation (promotion from DiscreteReal to Continuous) for all specified discrete real variables Note: container will be empty when not relaxing variables
Friends

- class SharedVariablesData
- class boost::serialization::access

allow boost access to serialize this class

13.185.1 Detailed Description

The representation of a SharedVariablesData instance. This representation, or body, may be shared by multiple SharedVariablesData handle instances.

The SharedVariablesData/SharedVariablesDataRep pairs utilize a handle-body idiom (Coplien, Advanced C++).

13.185.2 Member Function Documentation

```cpp
void copy_rep ( SharedVariablesDataRep ∗svd_rep ) [private]
```

copy the data from svd_rep to the current representation

Deep copies are used when recasting changes the nature of a Variables set.

References SharedVariablesDataRep::activeVarsComps_totals, SharedVariablesDataRep::all_continuousIDs, SharedVariablesDataRep::all_continuousLabels, SharedVariablesDataRep::all_continuousTypes, SharedVariablesDataRep::all_discreteIntLabels, SharedVariablesDataRep::all_discreteIntTypes, SharedVariablesDataRep::all_discreteRealLabels, SharedVariablesDataRep::all_discreteRealTypes, SharedVariablesDataRep::all_discreteStringLabels, SharedVariablesDataRep::all_discreteStringTypes, SharedVariablesDataRep::all_relaxedDiscreteInt, SharedVariablesDataRep::all_RelaxedDiscreteReal, SharedVariablesDataRep::cvStart, SharedVariablesDataRep::divStart, SharedVariablesDataRep::drvStart, SharedVariablesDataRep::dsvStart, SharedVariablesDataRep::icvStart, SharedVariablesDataRep::idivStart, SharedVariablesDataRep::idrvStart, SharedVariablesDataRep::idsvStart, SharedVariablesDataRep::inactiveVarsComps_totals, SharedVariablesDataRep::numCV, SharedVariablesDataRep::numDIV, SharedVariablesDataRep::numDRV, SharedVariablesDataRep::numDSV, SharedVariablesDataRep::numICV, SharedVariablesDataRep::numIDIV, SharedVariablesDataRep::numIDRV, SharedVariablesDataRep::numIDSV, SharedVariablesDataRep::variablesComponents, SharedVariablesDataRep::variablesComps_totals, and SharedVariablesDataRep::variablesView.

13.185.3 Member Data Documentation

```cpp
SizetArray variablesComps_totals [private]
```

totals for variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.

This data reflects the variable counts as originally specified and is not altered by relaxation.

Referenced by SharedVariablesDataRep::aleatory_uncertain_counts(), SharedVariablesDataRep::all_counts(), SharedVariablesDataRep::components_to_totals(), SharedVariablesDataRep::copy_rep(), SharedVariablesDataRep::design_counts(), SharedVariablesDataRep::epistemic_uncertain_counts(), SharedVariablesDataRep::initialize_active_components(), SharedVariablesDataRep::initialize_all_ids(), SharedVariablesDataRep::initialize_components_totals(), SharedVariablesDataRep::initialize_inactive_components(), SharedVariablesDataRep::relax_nocategorical(), SharedVariablesDataRep::state_counts(), SharedVariablesDataRep::uncertain_counts(), and SharedVariablesDataRep::view_start_counts().
SizetArray activeVarsCompsTotals  [private]
totals for active variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.
This data reflects the variable counts as originally specified and is not altered by relaxation.
Referenced by SharedVariablesDataRep::copy_rep(), and SharedVariablesDataRep::initialize_active_components().

SizetArray inactiveVarsCompsTotals  [private]
totals for inactive variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.
This data reflects the variable counts as originally specified and is not altered by relaxation.
Referenced by SharedVariablesDataRep::copy_rep(), and SharedVariablesDataRep::initialize_inactive_components().

SizetMultiArray allContinuousIds  [private]
array of 1-based position identifiers for the all continuous variables array
These identifiers define positions of the all continuous variables array within the total variable sequence. A primary use case is for defining derivative ids (DVV) based on an active subset.
Referenced by SharedVariablesDataRep::copy_rep(), and SharedVariablesDataRep::initialize_all_ids().
The documentation for this class was generated from the following files:
- SharedVariablesData.hpp
- SharedVariablesData.cpp

13.186 SimulationModel Class Reference

Derived model class which utilizes a simulation-based application interface to map variables into responses.
Inheritance diagram for SimulationModel:

```
Model

SimulationModel
```

Public Member Functions
- SimulationModel (ProblemDescDB &problem_db)
  constructor
- ~SimulationModel ()
  destructor

Protected Member Functions
- Interface & derived_interface ()
  return userDefinedInterface
- size_t solution_levels () const
return size of solnControlCostMap

- void solution_level_index (size_t lev_index)
  activate entry in solnControlCostMap

- RealVector solution_level_cost () const
  return cost estimates from solnControlCostMap

- void derived_evaluate (const ActiveSet &set)
  portion of evaluate() specific to SimulationModel (invokes a synchronous map() on userDefinedInterface)

- void derived_evaluate_nowait (const ActiveSet &set)
  portion of evaluate_nowait() specific to SimulationModel (invokes an asynchronous map() on userDefinedInterface)

- const IntResponseMap & derived_synchronize ()
  portion of synchronize() specific to SimulationModel (invokes synch() on userDefinedInterface)

- const IntResponseMap & derived_synchronize_nowait ()
  portion of synchronize_nowait() specific to SimulationModel (invokes synch_nowait() on userDefinedInterface)

- void component_parallel_mode (short mode)
  SimulationModel only supports parallelism in userDefinedInterface, so this virtual function redefinition is simply a
  sanity check.

- short local_eval_synchronization ()
  return userDefinedInterface synchronization setting

- int local_eval_concurrency ()
  return userDefinedInterface asynchronous evaluation concurrency

- bool derived_master_overload () const
  flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to userDefined-
  Interface)

- IntIntPair estimate_partition_bounds (int max_eval_concurrency)
  estimate the minimum and maximum partition sizes that can be utilized by this Model

- void derived_initCommunicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  set up SimulationModel for parallel operations (request forwarded to userDefinedInterface)

- void derived_init_serial ()
  set up SimulationModel for serial operations (request forwarded to userDefinedInterface).

- void derived_setCommunicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)
  set active parallel configuration for the SimulationModel (request forwarded to userDefinedInterface)

- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)
  Service userDefinedInterface job requests received from the master. Completes when a termination message is
  received from stop_servers().

- void stop_servers ()
  executed by the master to terminate userDefinedInterface server operations when SimulationModel iteration is
  complete.

- const String & interface_id () const
  return the userDefinedInterface identifier

- int derived_evaluation_id () const
  return the current evaluation id (simModelEvalCntr)

- bool evaluation_cache (bool recurse_flag=true) const
  return flag indicated usage of an evaluation cache by the SimulationModel (request forwarded to userDefined-
  Interface)
13.186. SIMULATIONMODEL CLASS REFERENCE

- bool `restart_file` (bool recurse_flag=true) const
  
  return flag indicated usage of a restart file by the SimulationModel (request forwarded to userDefinedInterface)

- void `set_evaluation_reference` ()
  
  set the evaluation counter reference points for the SimulationModel (request forwarded to userDefinedInterface)

- void `fine_grained_evaluation_counters` ()
  
  request fine-grained evaluation reporting within the userDefinedInterface

- void `print_evaluation_summary` (std::ostream &s, bool minimal_header=false, bool relative_count=true) const
  
  print the evaluation summary for the SimulationModel (request forwarded to userDefinedInterface)

- void `eval_tag_prefix` (const String &eval_id_str)
  
  set the hierarchical eval ID tag prefix

**Private Member Functions**

- void `initialize_solution_control` (const String &control, const RealVector &cost)
  
  process the solution level inputs to define solnControlVarIndex, solnControlVarType, and solnControlCostMap

**Private Attributes**

- Interface `userDefinedInterface`
  
  the interface used for mapping variables to responses

- short `solnCntlVarType`
  
  type of the discrete variable that controls the set/range of solution levels

- size_t `solnCntlADVIndex`
  
  index of the discrete variable (within all view) that controls the set/range of solution levels

- size_t `solnCntlSetIndex`
  
  index of the discrete set variable (within its type array, managing offset when solnCntlVarType is a subset of all discrete variables) that controls the set/range of solution levels

- std::map<Real, size_t> `solnCntlCostMap`
  
  sorted array of relative costs associated with a set of solution levels

- size_t `simModelEvalCntr`
  
  counter for calls to derived_evaluate()/derived_evaluate_nowait()

- IntIntMap `simIdMap`
  
  map from userDefinedInterface evaluation ids to SimulationModel ids (may differ in case where the same interface instance is shared by multiple models)

- IntResponseMap `simResponseMap`
  
  map of simulation-based responses returned by derived_synchronize() and derived_synchronize_nowait()

**Additional Inherited Members**

13.186.1 Detailed Description

Derived model class which utilizes a simulation-based application interface to map variables into responses.

The SimulationModel class is the simplest of the derived model classes. It provides the capabilities of the original Model class, prior to the development of surrogate and nested model extensions. The derived response computation and synchronization functions utilize an application interface to perform the function evaluations.
13.186.2 Member Function Documentation

void eval_tag_prefix ( const String & eval_id_str ) [protected], [virtual]

set the hierarchical eval ID tag prefix
SimulationModel doesn’t need to change the tagging, so just forward to Interface
Reimplemented from Model.
References Interface::eval_tag_prefix(), and SimulationModel::userDefinedInterface.
The documentation for this class was generated from the following files:
- SimulationModel.hpp
- SimulationModel.cpp

13.187 SimulationResponse Class Reference

Container class for response functions and their derivatives. SimulationResponse provides the body class.
Inheritance diagram for SimulationResponse:

```
  Response
     |     
  +------------------
  |                  
SimulationResponse
```

Public Member Functions

- SimulationResponse ()
  default constructor
- SimulationResponse (const Variables &vars, const ProblemDescDB &problem_db)
  standard constructor built from problem description database
- SimulationResponse (const SharedResponseData &srd, const ActiveSet &set)
  alternate constructor that shares a SharedResponseData instance
- SimulationResponse (const SharedResponseData &srd)
  alternate constructor that shares a SharedResponseData instance
- SimulationResponse (const ActiveSet &set)
  alternate constructor using limited data
- ~SimulationResponse ()
  destructor

Additional Inherited Members

13.187.1 Detailed Description

Container class for response functions and their derivatives. SimulationResponse provides the body class.
The SimulationResponse class is the "representation" of the response container class. It is the "body" portion
of the "handle-body idiom" (see Coplien "Advanced C++", p. 58). The handle class (Response) provides for
memory efficiency in management of multiple response objects through reference counting and representation
sharing. The body class (SimulationResponse) actually contains the response data (functionValues, function- 
Gradients, functionHessians, etc.). The representation is hidden in that an instance of SimulationResponse may 
only be created by Response. Therefore, programmers create instances of the Response handle class, and only 
need to be aware of the handle/body mechanisms when it comes to managing shallow copies (shared representa-
tion) versus deep copies (separate representation used for history mechanisms).

The documentation for this class was generated from the following files:

- SimulationResponse.hpp
- SimulationResponse.cpp

13.188 SNLLBase Class Reference

Base class for OPT++ optimization and least squares methods.

Inheritance diagram for SNLLBase:

```
    SNLLBase
     |            +-- SNLLLeastSq
     |                  +-- SNLLOptimizer
```

Public Member Functions

- **SNLLBase ()**
  - default constructor

- **SNLLBase (ProblemDescDB &problem_db)**
  - standard constructor

- **~SNLLBase ()**
  - destructor

Protected Member Functions

- void **copy_con_vals_dak_to_optpp** (const RealVector &local_fn_vals, RealVector &g, size_t offset)
  - convenience function for copying local_fn_vals to g; used by constraint evaluator functions

- void **copy_con_vals_optpp_to_dak** (const RealVector &g, RealVector &local_fn_vals, size_t offset)
  - convenience function for copying g to local_fn_vals; used in final solution logging

- void **copy_con_grad** (const RealMatrix &local_fn_grads, RealMatrix &grad_g, size_t offset)
  - convenience function for copying local_fn_grads to grad_g; used by constraint evaluator functions

- void **copy_con_hess** (const RealSymMatrixArray &local_fn_hessians, OPTPP::OptppArray<RealSymMatrix> &hess_g, size_t offset)
  - convenience function for copying local_fn_hessians to hess_g; used by constraint evaluator functions

- void **snll_pre_instantiate** (bool bound_constr_flag, int num_constr)
  - convenience function for setting OPT++ options prior to the method instantiation

- void **snll_post_instantiate** (int num_cv, bool vendor_num_grad_flag, const String &finite_diff_type, const RealVector &fdss, int max_iter, int max_fn_evals, Real conv_tol, Real grad_tol, Real max_step, bool bound_constr_flag, int num_constr, short output_level, OPTPP::OptimizeClass *the_optimizer, OPTPP::NLP0 *nlf_objective, OPTPP::FDNLF1 *fd_nlf1, OPTPP::FDNLF1 *fd_nlf1_con)
  -
convenience function for setting OPT++ options after the method instantiation

- void snll_initialize_run (OPTPP::NLP0 *nlf_objective, OPTPP::NLP *nlp_constraint, const RealVector &init_pt, bool bound_constr_flag, const RealVector &lower_bnds, const RealVector &upper_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_l_bnds, const RealVector &lin_eq_u_bnds, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_l_bnds, const RealVector &nln_eq_u_bnds)

convenience function for OPT++ configuration prior to the method invocation

- void snll_post_run (OPTPP::NLP0 *nlf_objective)

convenience function for setting OPT++ options after the method instantiations

Static Protected Member Functions

- static void init_fn (int n, RealVector &x)

An initialization mechanism provided by OPT++ (not currently used).

Protected Attributes

- String searchMethod
  value_based_line_search, gradient_based_line_search, trust_region, or tr_pds
- OPTPP::SearchStrategy searchStrat
  enum: LineSearch, TrustRegion, or TrustPDS
- OPTPP::MeritFcn meritFn
  enum: NormFmu, ArgaezTapia, or VanShanno
- Real maxStep
  value from max_step specification
- Real stepLenToBndry
  value from steplength_to_boundary specification
- Real centeringParam
  value from centering parameter specification
- bool constantASVFlag
  flags a user selection of active_set_vector == constant. By mapping this into mode override, reliance on duplicate detection can be avoided.

Static Protected Attributes

- static Minimizer * optLSqInstance
  pointer to the active base class object instance used within the static evaluator functions in order to avoid the need for static data
- static bool modeOverrideFlag
  flags OPT++ mode override (for combining value, gradient, and Hessian requests)
- static EvalType lastFnEvalLocn
  an enum used to track whether an nlf evaluator or a constraint evaluator was the last location of a function evaluation
- static int lastEvalMode
  copy of mode from constraint evaluators
- static RealVector lastEvalVars
  copy of variables from constraint evaluators
13.189. SNLLLEASTSQ CLASS REFERENCE

13.188.1 Detailed Description

Base class for OPT++ optimization and least squares methods.

The SNLLBase class provides a common base class for SNLLOptimizer and SNLLLeastSq, both of which are wrappers for OPT++, a C++ optimization library from the Computational Sciences and Mathematics Research (CSMR) department at Sandia’s Livermore CA site.

The documentation for this class was generated from the following files:

- SNLLBase.hpp
- SNLLBase.cpp

13.189 SNLLLeastSq Class Reference

Wrapper class for the OPT++ optimization library.

Inheritance diagram for SNLLLeastSq:

```
+--- Iterator
    +--- Minimizer
    |    +--- LeastSq
    |    |    +--- SNLLBase
    |    |    |    +--- SNLLLeastSq
```

Public Member Functions

- **SNLLLeastSq (ProblemDescDB &problem_db, Model &model)**
  
  standard constructor

- **SNLLLeastSq (const String &method_name, Model &model)**
  
  alternate constructor for instantiations without ProblemDescDB support

- **~SNLLLeastSq ()**
  
  destructor

- **void core_run ()**
  
  compute the least squares solution

Protected Member Functions

- **void initialize_run ()**
  
  invokes LeastSq::initialize_run(), SNLLBase::snll_initialize_run(), and performs other set-up

- **void post_run (std::ostream &s)**
  
  invokes snll_post_run and re-implements post_run (does not call parent) and performs other solution processing

- **void finalize_run ()**
  
  restores instances
Static Private Member Functions

- static void *nlf2_evaluator_gn (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, RealSymMatrix &hess_f, int &result_mode)
  
  objective function evaluator function which obtains values and gradients for least square terms and computes
  objective function value, gradient, and Hessian using the Gauss-Newton approximation.

- static void constraint1_evaluator_gn (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
  
  constraint evaluator function which provides constraint values and gradients to OPT++ Gauss-Newton methods.

- static void constraint2_evaluator_gn (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, OPTPP::OptppArray<RealSymMatrix> &hess_g, int &result_mode)
  
  constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ Gauss-Newton
  methods.

Private Attributes

- SNLLLeastSq * prevSnllLSqInstance
  
  pointer to the previously active object instance used for restoration in the case of iterator/model recursion

- OPTPP::NLP0 * nlfObjective
  
  objective NLF base class pointer

- OPTPP::NLP0 * nlfConstraint
  
  constraint NLF base class pointer

- OPTPP::NLP * nlpConstraint
  
  constraint NLP pointer

- OPTPP::NLF2 * nlf2
  
  pointer to objective NLF for full Newton optimizers

- OPTPP::NLF2 * nlf2Con
  
  pointer to constraint NLF for full Newton optimizers

- OPTPP::NLF1 * nlf1Con
  
  pointer to constraint NLF for Quasi Newton optimizers

- OPTPP::OptimizeClass * theOptimizer
  
  optimizer base class pointer

- OPTPP::OptNewton * optnewton
  
  Newton optimizer pointer.

- OPTPP::OptBCNewton * optbcnewton
  
  Bound constrained Newton optimizer ptr.

- OPTPP::OptDHNIPS * optdhnips
  
  Disaggregated Hessian NIPS optimizer ptr.

Static Private Attributes

- static SNLLLeastSq * snllLSqInstance
  
  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static
data
Additional Inherited Members

13.189.1 Detailed Description

Wrapper class for the OPT++ optimization library.

The SNLLLeastSq class provides a wrapper for OPT++, a C++ optimization library of nonlinear programming and pattern search techniques from the Computational Sciences and Mathematics Research (CSMR) department at Sandia’s Livermore CA site. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function, a static member, or accessed by static pointer.

The user input mappings are as follows: max_iterations, max_function_evaluations, convergence_tolerance, max_step, gradient_tolerance, search_method, and search_scheme_size are set using OPT++’s setMaxIter(), setMaxFeval(), setFcnTol(), setMaxStep(), setGradTol(), setSearchStrategy(), and setSSS() member functions, respectively; output verbosity is used to toggle OPT++’s debug mode using the setDebug() member function. Internal to OPT++, there are 3 search strategies, while the DAKOTA search_method specification supports 4 (value_based_line_search, gradient_based_line_search, trust_region, or tr_pds). The difference stems from the “is_expensive” flag in OPT++. If the search strategy is LineSearch and “is_expensive” is turned on, then the value_based_line_search is used. Otherwise (the “is_expensive” default is off), the algorithm will use the gradient_based_line_search. Refer to [Meza, J.C., 1994] and to the OPT++ source in the Dakota/packages/OPTPP directory for information on OPT++ class member functions.

13.189.2 Member Function Documentation

void post_run ( std::ostream & s ) [protected], [virtual]
invokes snll_post_run and re-implements post_run (does not call parent) and performs other solution processing.

SNLLLeastSq requires fn DB lookup, so overrides LeastSq::post_run and directly invokes Iterator::post_run when complete.

Reimplemented from LeastSq.

References Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, SNLLBase::copy_const_vals_optpp_to_dak(), Dakota::copy_data_partial(), Dakota::data_pairs, LeastSq::get_confidence_intervals(), Model::interface_id(), Iterator::iteratedModel, Dakota::lookup_by_val(), Model::model_rep(), SNLLLeastSq::nlfObjective, Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, Minimizer::post_run(), ActiveSet::request_vector(), Minimizer::scaleFlag, Minimizer::scalingModel, SNLLBase::snll_post_run(), and SNLLLeastSq::the_Optimizer.

void nlf2_evaluator_gn ( int mode, int n, const RealVector & x, double & f, RealVector & grad_f, RealSymMatrix & hess_f, int & result_mode ) [static], [private]
optimisation function evaluator function which obtains values and gradients for least square terms and computes objective function value, gradient, and Hessian using the Gauss-Newton approximation.

This nlf2 evaluator function is used for the Gauss-Newton method in order to exploit the special structure of the nonlinear least squares problem. Here, \( f_x = \sum (T_i - Tbar_i)^2 \) and Response is made up of residual functions and their gradients along with any nonlinear constraints. The objective function and its gradient vector and Hessian matrix are computed directly from the residual functions and their derivatives (which are returned from the Response object).

References Dakota::abort_handler(), Iterator::activeSet, Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnevalLocn, Minimizer::numFunctions, Least-
void constraint1_evaluator_gn ( int mode, int n, const RealVector & x, RealVector & g, RealMatrix & grad_g, int & result_mode ) [static], [private]

constraint evaluator function which provides constraint values and gradients to OPT++ Gauss-Newton methods.

While it does not employ the Gauss-Newton approximation, it is distinct from constraint1_evaluator() due to its need to anticipate the required modes for the least squares terms. This constraint evaluator function is used with diaggregated Hessian NIPS and is currently active.

References Dakota::abort_handler(), Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numFunctions, LeastSq::numLeastSqTerms, Iterator::outputLevel, ActiveSet::request_vector(), and SNLLLeastSq::snllLSqInstance.

Referenced by SNLLLeastSq::SNLLLeastSq().

void constraint2_evaluator_gn ( int mode, int n, const RealVector & x, RealVector & g, RealMatrix & grad_g, OPTPP::OptppArray<RealSymMatrix> & hess_g, int & result_mode ) [static], [private]

constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ Gauss-Newton methods.

While it does not employ the Gauss-Newton approximation, it is distinct from constraint2_evaluator() due to its need to anticipate the required modes for the least squares terms. This constraint evaluator function is used with full Newton NIPS and is currently inactive.

References Dakota::abort_handler(), Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy_con_hess(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_hessians(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, SNLLBase::modeOverrideFlag, Minimizer::numFunctions, LeastSq::numLeastSqTerms, Iterator::outputLevel, ActiveSet::request_vector(), and SNLLLeastSq::snllLSqInstance.

The documentation for this class was generated from the following files:

- SNLLLeastSq.hpp
- SNLLLeastSq.cpp

13.190  SNLLOptimizer Class Reference

Wrapper class for the OPT++ optimization library.

Inheritance diagram for SNLLOptimizer:
Public Member Functions

- **SNLLOptimizer (ProblemDescDB &problem_db, Model &model)**
  
  *standard constructor*

- **SNLLOptimizer (const String &method_string, Model &model)**
  
  *alternate constructor for instantiations "on the fly"*

- **SNLLOptimizer (const RealVector &initial_pt, const RealVector &var_l_bnds, const RealVector &var_u_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_tgts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, void(*user_obj_eval)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode), void(*user_con_eval)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode))**

  *alternate constructor for instantiations "on the fly"*

- **∼SNLLOptimizer ()**
  
  *destructor*

- **void core_run ()**
  
  *Performs the iterations to determine the optimal solution.*

Protected Member Functions

- **void initialize_run ()**
  
  *invokes Optimizer::initialize_run(), SNLLBase::snll_initialize_run(), and performs other set-up*

- **void post_run (std::ostream &s)**
  
  *performs data recovery and calls Optimizer::post_run()*

- **void finalize_run ()**
  
  *performs cleanup, restores instances and calls parent finalize*

Private Member Functions

- **void default_instantiate_q_newton (void(*obj_eval)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode), void(*con_eval)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode))**

  *instantiate an OPTPP.Q_NEWTON solver using standard settings*
- void default_instantiate_newton (void(*obj_eval)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, RealSymMatrix &hess_f, int &result_mode), void(*con_eval)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, OPTPP::OptppArray<RealSymMatrix> &hess_g, int &result_mode))
  
  instantiate an OPTPP_NEWTON solver using standard settings

Static Private Member Functions

- static void nlf0_evaluator (int n, const RealVector &x, double &f, int &result_mode)
  
  objective function evaluator function for OPT++ methods which require only function values.

- static void nlf1_evaluator (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)
  
  objective function evaluator function which provides function values and gradients to OPT++ methods.

- static void nlf2_evaluator (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, RealSymMatrix &hess_f, int &result_mode)
  
  objective function evaluator function which provides function values, gradients, and Hessians to OPT++ methods.

- static void constraint0_evaluator (int n, const RealVector &x, RealVector &g, int &result_mode)
  
  constraint evaluator function for OPT++ methods which require only constraint values.

- static void constraint1_evaluator (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
  
  constraint evaluator function which provides constraint values and gradients to OPT++ methods.

- static void constraint2_evaluator (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, OPTPP::OptppArray<RealSymMatrix> &hess_g, int &result_mode)
  
  constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ methods.

Private Attributes

- SNLLOptimizer * prevSnllOptInstance
  
  pointer to the previously active object instance used for restoration in the case of iterator/model recursion

- OPTPP::NLP0 * nlfObjective
  
  objective NLF base class pointer

- OPTPP::NLP0 * nlfConstraint
  
  constraint NLF base class pointer

- OPTPP::NLP * nlpConstraint
  
  constraint NLP pointer

- OPTPP::NLF0 * nlf0
  
  pointer to objective NLF for nongradient optimizers

- OPTPP::NLF1 * nlf1
  
  pointer to objective NLF for (analytic) gradient-based optimizers

- OPTPP::NLF1 * nlf1Con
  
  pointer to constraint NLF for (analytic) gradient-based optimizers

- OPTPP::FDNLF1 * fdnlf1
  
  pointer to objective NLF for (finite diff) gradient-based optimizers

- OPTPP::FDNLF1 * fdnlf1Con
  
  pointer to constraint NLF for (finite diff) gradient-based optimizers
Static Private Attributes

- **SNLLOptimizer** * snlOptInstance
  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data.
Additional Inherited Members

13.190.1 Detailed Description

Wrapper class for the OPT++ optimization library.

The SNLLOptimizer class provides a wrapper for OPT++, a C++ optimization library of nonlinear programming and pattern search techniques from the Computational Sciences and Mathematics Research (CSMR) department at Sandia’s Livermore CA site. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function, a static member, or accessed by static pointer.

The user input mappings are as follows: max_iterations, max_function_evaluations, convergence_tolerance, max_step, gradient_tolerance, search_method, and search_scheme_size are set using OPT++’s setMaxIter(), setMaxEval(), setFcnTol(), setMaxStep(), setGradTol(), setSearchStrategy(), and setSSS() member functions, respectively; output verbosity is used to toggle OPT++’s debug mode using the setDebug() member function. Internal to OPT++, there are 3 search strategies, while the DAKOTA search_method specification supports 4 (value_based_line_search, gradient_based_line_search, trust_region, or tr_pds). The difference stems from the “is_expensive” flag in OPT++. If the search strategy is LineSearch and “is_expensive” is turned on, then the value_based_line_search is used. Otherwise (the “is_expensive” default is off), the algorithm will use the gradient_based_line_search. Refer to [Meza, J.C., 1994] and to the OPT++ source in the Dakota/packages/OPTPP directory for information on OPT++ class member functions.

13.190.2 Constructor & Destructor Documentation

SNLLOptimizer ( ProblemDescDB & problem_db, Model & model )

standard constructor

This constructor is used for normal instantiations using data from the ProblemDescDB.

References Dakota::abort_handler(), Minimizer::boundConstraintFlag, SNLLBase::centeringParam, SNLLOptimizer::constraint0_evaluator(), SNLLOptimizer::constraint1_evaluator(), SNLLOptimizer::constraint2_evaluator(), Iterator::convergenceTol, SNLLOptimizer::default_instantiate_newton(), SNLLOptimizer::default_instantiate_q_newton(), Model::fd_gradient_step_size(), SNLLOptimizer::fdnlf1(), SNLLOptimizer::fdnlf1Con, ProblemDescDB::get_int(), ProblemDescDB::get_real(), SNLLBase::init_fn(), Model::interval_type(), Iterator::iteratedModel, Dakota::LARGE_SCALE, Iterator::maxEvalConcurrency, Iterator::maxFunctionEvals, Iterator::maxIterations, SNLLBase::maxStep, SNLLBase::init_fn(), Iterator::method_enum_to_string(), Iterator::methodName, SNLLOptimizer::nlf0, SNLLOptimizer::nlf0_evaluator(), SNLLOptimizer::nlf1, SNLLOptimizer::nlf1_evaluator(), SNLLOptimizer::nlf1Con, SNLLOptimizer::nlf2_evaluator(), SNLLOptimizer::nlfConstraint, SNLLOptimizer::nlfObjective, SNLLOptimizer::nlpConstraint, Minimizer::numConstraints, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, SNLLOptimizer::optbcfstdnewton, SNLLOptimizer::optbcqnewton, SNLLOptimizer::optcgm, SNLLOptimizer::optdfnewton, SNLLOptimizer::optdfnips, SNLLOptimizer::optlbfgs, SNLLOptimizer::optpds, SNLLOptimizer::optqnewton, SNLLOptimizer::optqnips, Iterator::outputLevel, Iterator::probDescDB, SNLLBase::searchStrat, SNLLBase::snll_post_instantiate(), SNLLBase::snll_pre_instantiate(), SNLLBase::stepLenToBndry, SNLLOptimizer::theOptimizer, and Minimizer::vendorNumericalGradFlag.

SNLLOptimizer ( const String & method_string, Model & model )

alternate constructor for instantiations ”on the fly”

This is an alternate constructor for instantiations on the fly using a Model but no ProblemDescDB.

References Dakota::abort_handler(), Minimizer::boundConstraintFlag, SNLLOptimizer::constraint1_evaluator(), SNLLOptimizer::constraint2_evaluator(), Iterator::convergenceTol, SNLLOptimizer::default_instantiate_newton(),
SNLLOptimizer (const RealVector &initial_pt, const RealVector &var_l_bnds, const RealVector &var_u_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq tgts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq tgts, void(*)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode) user_obj_eval, void(*)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode) user_con_eval)

This is an alternate constructor for performing an optimization using the passed in objective function and constraint function pointers.

References Minimizer::bigRealBoundSize, Minimizer::boundConstraintFlag, SNLLOptimizer::default_instantiate_q_newton(), SNLLOptimizer::initializeRun, SNLLOptimizer::initialPoint, SNLLOptimizer::lowerBounds, SNLLOptimizer::nloObjective, SNLLOptimizer::nlpConstraint, Minimizer::numConstraints, Minimizer::numContinuousVars, Iterator::outputLevel, SNLLBase::snllPostInstantiate(), SNLLOptimizer::theOptimizer, and SNLLOptimizer::upperBounds.

### 13.190.3 Member Function Documentation

**void nlf0_evaluator ( int n, const RealVector &x, double &f, int &result_mode )**  [static], [private]

Objective function evaluator function for OPT++ methods which require only function values.

For use when DAKOTA computes f and gradients are not directly available. This is used by nongradient-based optimizers such as PDS and by gradient-based optimizers in vendor numerical gradient mode (opt++’s internal finite difference routine is used).

References Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_value(), Iterator::iteratedModel, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numNonlinearConstraints, Iterator::outputLevel, Model::primary_response_fn_sense(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

**void nlf1_evaluator ( int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode )**  [static], [private]

Objective function evaluator function which provides function values and gradients to OPT++ methods.

For use when DAKOTA computes f and df/dX (regardless of gradient type). Vendor numerical gradient case is handled by nlf0_evaluator.

References Iterator::activeSet, Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_gradient_copy(), Response::function_value(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numNonlinearConstraints, Iterator::outputLevel, Model::primary_response_fn_sense(), ActiveSet::request_values(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().
void nlf2_evaluator ( int mode, int n, const RealVector & x, double & f, RealVector & grad_f, RealSymMatrix & hess_f, int & result_mode ) [static], [private]

objective function evaluator function which provides function values, gradients, and Hessians to OPT++ methods.

For use when DAKOTA receives f, df/dX, & d^2f/dx^2 from the ApplicationInterface (analytic only). Finite differencing does not make sense for a full Newton approach, since lack of analytic gradients & Hessian should dictate the use of quasi-newton or fd-newton. Thus, there is no fdnlf2_evaluator for use with full Newton approaches, since it is preferable to use quasi-newton or fd-newton with nlf1. Gauss-Newton does not fit this model; it uses nlf2_evaluator_gn instead of nlf2_evaluator.

References Iterator::activeSet, Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_gradient_copy(), Response::function_hessian(), Response::function_value(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numNonlinearConstraints, Iterator::outputLevel, Model::primary_response_fn_sense(), ActiveSet::request_values(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

void constraint0_evaluator ( int n, const RealVector & x, RealVector & g, int & result_mode ) [static], [private]

constraint evaluator function for OPT++ methods which require only constraint values.

For use when DAKOTA computes g and gradients are not directly available. This is used by nongradient-based optimizers and by gradient-based optimizers in vendor numerical gradient mode (OPT++’s internal finite difference routine is used).

References Model::continuous_variables(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Optimizer::numObjectiveFns, Iterator::outputLevel, and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

void constraint1_evaluator ( int mode, int n, const RealVector & x, RealVector & g, RealMatrix & grad_g, int & result_mode ) [static], [private]

constraint evaluator function which provides constraint values and gradients to OPT++ methods.

For use when DAKOTA computes g and dg/dX (regardless of gradient type). Vendor numerical gradient case is handled by constraint0_evaluator.

References Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Optimizer::numObjectiveFns, Iterator::outputLevel, ActiveSet::request_values(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

void constraint2_evaluator ( int mode, int n, const RealVector & x, RealVector & g, RealMatrix & grad_g, OPTPP::OptppArray<RealSymMatrix> & hess_g, int & result_mode ) [static], [private]

constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ methods.

For use when DAKOTA computes g, dg/dX, & d^2g/dx^2 (analytic only).

References Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy_con_hess(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_hessians(), Response::function_values(), Iterator::iteratedModel, SNLL-
13.191 SOLBase Class Reference

Base class for Stanford SOL software.

Inheritance diagram for SOLBase:

```
SOLBase
  NLSSOLLeastSq
  NPSOLOptimizer
```

Public Member Functions

- **SOLBase ()**
  
  *default constructor*

- **SOLBase (Model &model)**
  
  *standard constructor*

- **~SOLBase ()**
  
  *destructor*

Protected Member Functions

- **void allocate_arrays (int num_cv, int_t num_nln_con, const RealMatrix &lin_ineq_coeffs, const RealMatrix &lin_eq_coeffs)**

  *Allocates miscellaneous arrays for the SOL algorithms.*

- **void deallocate_arrays ()**

  *Deallocation memory previously allocated by allocate_arrays().*

- **void allocate_workspace (int num_cv, int_t num_nln_con, int_t num_lin_con, int_t num_lsq)**

  *Allocates real and integer workspaces for the SOL algorithms.*

- **void set_options (bool speculative_flag, bool vendor_num_grad_flag, short output_level, int verify_level, Real fn_prec, Real linesrch_tol, int max_iter, Real constr_tol, Real conv_tol, const std::string &grad_type, const RealVector &fdss)**

  *Sets SOL method options using calls to npsoptn2.*

- **void augment_bounds (RealVector &augmented_l_bnds, RealVector &augmented_u_bnds, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealVector &lin_eq_targets, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_targets)**

  *Augments variable bounds with linear and nonlinear constraint bounds.*
**Static Protected Member Functions**

- static void `constraint_eval` (int &mode, int &ncnln, int &n, int &nrowj, int *needc, double *x, double *c, double *cjac, int &nstate)

  *CONFUN in NPSOL manual: computes the values and first derivatives of the nonlinear constraint functions.*

**Protected Attributes**

- int `realWorkSpaceSize`
  
  *size of realWorkSpace*

- int `intWorkSpaceSize`
  
  *size of intWorkSpace*

- `RealArray realWorkSpace`
  
  *real work space for NPSOL/NLSSOL*

- `IntArray intWorkSpace`
  
  *int work space for NPSOL/NLSSOL*

- int `nlnConstraintArraySize`
  
  *used for non-zero array sizing (nonlinear constraints)*

- int `linConstraintArraySize`
  
  *used for non-zero array sizing (linear constraints)*

- `RealArray cLambda`
  
  *CLAMBDA from NPSOL manual: Langrange multipliers.*

- `IntArray constraintState`
  
  *ISTATE from NPSOL manual: constraint status.*

- int `informResult`
  
  *INFORM from NPSOL manual: optimization status on exit.*

- int `numberIterations`
  
  *ITER from NPSOL manual: number of (major) iterations performed.*

- int `boundsArraySize`
  
  *length of augmented bounds arrays (variable bounds plus linear and nonlinear constraint bounds)*

- double * `linConstraintMatrixF77`
  
  *[A] matrix from NPSOL manual: linear constraint coefficients*

- double * `upperFactorHessianF77`
  

- double * `constraintJacMatrixF77`
  
  *[CJAC] matrix from NPSOL manual: nonlinear constraint Jacobian*

- int `fnEvalCntr`
  
  *counter for testing against maxFunctionEvals*

- size_t `constrOffset`
  
  *used in `constraint_eval()` to bridge NLSSOLLeastSq::numLeastSqTerms and NPSOLOptimizer::numObjectiveFns*
### Static Protected Attributes

- static SOLBase * solInstance
  
  *pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data*

- static Minimizer * optLsqInstance
  
  *pointer to the active base class object instance used within the static evaluator functions in order to avoid the need for static data*

### 13.191.1 Detailed Description

Base class for Stanford SOL software.

The SOLBase class provides a common base class for NPSOLOptimizer and NLSSOLLeastSq, both of which are Fortran 77 sequential quadratic programming algorithms from Stanford University marketed by Stanford Business Associates.

The documentation for this class was generated from the following files:

- SOLBase.hpp
- SOLBase.cpp

### 13.192 SpawnApplicInterface Class Reference

Derived application interface class which spawns simulation codes using spawnvp.

Inheritance diagram for SpawnApplicInterface:

```
    Interface
     |
     v
  ApplicationInterface
     |
     v
ProcessApplicInterface
     |
     v
ProcessHandleApplicInterface
     |
     v
SpawnApplicInterface
```

#### Public Member Functions

- **SpawnApplicInterface (const ProblemDescDB &problem_db)**
  
  *constructor*

- **~SpawnApplicInterface ()**
  
  *destructor*
Protected Member Functions

- void wait_local_evaluations (PRPQueue &prp_queue)
  
  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.

- void test_local_evaluations (PRPQueue &prp_queue)
  
  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version is nonblocking and will return without any completions if none are immediately available.

- pid_t create_analysis_process (bool block_flag, bool new_group)
  
  spawn a child process for an analysis component within an evaluation

- size_t wait_local_analyses ()
  
  wait for asynchronous analyses on the local processor, completing at least one job

- size_t test_local_analyses_send (int analysis_id)
  
  test for asynchronous analysis completions on the local processor and return results for any completions by sending messages

Additional Inherited Members

13.192.1 Detailed Description

Derived application interface class which spawns simulation codes using spawnvp. SpawnApplicInterface is used on Windows systems and is a peer to ForkApplicInterface for Unix systems. The documentation for this class was generated from the following files:

- SpawnApplicInterface.hpp
- SpawnApplicInterface.cpp

13.193 SurfpackApproximation Class Reference

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota. Inheritance diagram for SurfpackApproximation:

```
+----------------+     +----------------+     +----------------+
|                | ---+ |                | ---+ |                |
|                v    |                v    |                v    
| SurfpackApproximation  +-------+ Approximation +-------+ Dakota |
```

Public Member Functions

- SurfpackApproximation ()
  
  default constructor

- SurfpackApproximation (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)
  
  standard constructor: Surfpack surface of appropriate type will be created

- SurfpackApproximation (const SharedApproxData &shared_data)
Protected Member Functions

- **int min_coefficients () const**
  
  *return the minimum number of samples (unknowns) required to build the derived class approximation type in num-Vars dimensions*

- **int recommended_coefficients () const**
  
  *return the recommended number of samples (unknowns) required to build the derived class approximation type in numVars dimensions*

- **void build ()**
  
  *SurfData object will be created from Dakota’s SurrogateData, and the appropriate Surfpack build method will be invoked.*

- **void export_model (const String &fn_label, const String &export_prefix="", const unsigned short export_format=NOMODEL_FORMAT)**
  
  *export the Surpack model to disk or console*

- **Real value (const Variables &vars)**
  
  *Return the value of the Surfpack surface for a given parameter vector x.*

- **const RealVector & gradient (const Variables &vars)**
  
  *retrieve the approximate function gradient for a given parameter vector x*

- **const RealSymMatrix & hessian (const Variables &vars)**
  
  *retrieve the approximate function Hessian for a given parameter vector x*

- **Real prediction_variance (const Variables &vars)**
  
  *retrieve the variance of the predicted value for a given parameter set x (KrigingModel only)*

- **Real value (const RealVector &c_vars)**
  
  *Return the value of the Surfpack surface for a given parameter vector x.*

- **const RealVector & gradient (const RealVector &c_vars)**
  
  *retrieve the approximate function gradient for a given parameter vector x*

- **const RealSymMatrix & hessian (const RealVector &c_vars)**
  
  *retrieve the approximate function Hessian for a given parameter vector x*

- **Real prediction_variance (const RealVector &c_vars)**
  
  *retrieve the variance of the predicted value for a given parameter set x (KrigingModel only)*

- **bool diagnostics_available ()**
  
  *check if the diagnostics are available (true for the Surfpack types)*

- **Real diagnostic (const String &metric_type)**
  
  *retrieve a single diagnostic metric for the diagnostic type specified on the primary model and data*

- **Real diagnostic (const String &metric_type, const SurfpackModel &model, const SurfData &data)**
  
  *retrieve a single diagnostic metric for the diagnostic type specified on the given model and data*

- **void primary_diagnostics (int fn_index)**
  
  *compute and print all requested diagnostics and cross-validation*

- **void challenge_diagnostics (int fn_index, const RealMatrix &challenge_points, const RealVector &challenge_responses)**
compute and print all requested diagnostics for user provided challenge pts

- **RealArray cv_diagnostic** (const StringArray &metric_types, unsigned num_folds)
  
  compute and return cross-validation for metric_type with num_folds

- **RealArray challenge_diagnostic** (const StringArray &metric_types, const RealMatrix &challenge_points, const RealVector &challenge_responses)
  
  compute and print all requested diagnostics for user provided challenge pts

### Private Member Functions

- **SurfData * surrogates_to_surf_data ()**
  
  copy from SurrogateData to SurfPoint/SurfData

- **void add_anchor_to_surfdata (SurfData &surf_data)**
  
  set the anchor point (including gradient and hessian if present) into surf_data

### Private Attributes

- **SurfpackModel * model**
  
  The native Surfpack approximation.

- **SurfpackModelFactory * factory**
  
  factory for the SurfpackModel instance

- **SurfData * surfData**
  
  The data used to build the approximation, in Surfpack format.

### Additional Inherited Members

#### 13.193.1 Detailed Description

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

The SurfpackApproximation class is the interface between Dakota and Surfpack. Based on the information in the ProblemDescDB that is passed in through the constructor, SurfpackApproximation builds a Surfpack Surface object that corresponds to one of the following data-fitting techniques: polynomial regression, kriging, artificial neural networks, radial basis function network, or multivariate adaptive regression splines (MARS).

#### 13.193.2 Constructor & Destructor Documentation

**SurfpackApproximation ( const ProblemDescDB & problem_db, const SharedApproxData & shared_data, const String & approx_label )**

standard constructor: Surfpack surface of appropriate type will be created

Initializes the embedded Surfpack surface object and configure it using the specifications from the input file.

Data for the surface is created later.

References Dakota::abort_handler(), SharedSurfpackApproxData::approxOrder, SharedApproxData::approxType, SharedApproxData::buildDataOrder, Dakota::copy_data(), SharedSurfpackApproxData::crossValidateFlag, SharedSurfpackApproxData::diagnosticSet, SurfpackApproximation::factory, ProblemDescDB::get_real(), ProblemDescDB::get_rv(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), SharedSurfpackApproxData::numFolds, SharedApproxData::numVars, SharedApproxData::outputLevel, SharedSurfpackApproxData::percentFold, and Approximation::sharedDataRep.
SurfpackApproximation (const SharedApproxData & shared_data)

alternate constructor
On-the-fly constructor which uses mostly Surfpack model defaults.
References Dakota::abort_handler(), SharedSurfpackApproxData::approxOrder, SharedApproxData::approxType, SharedApproxData::buildDataOrder, SurfpackApproximation::factory, SharedApproxData::numVars, SharedApproxData::outputLevel, and Approximation::sharedDataRep.

13.193.3 Member Function Documentation

void build ( ) [protected], [virtual]
SurfData object will be created from Dakota’s SurrogateData, and the appropriate Surfpack build method will be invoked.
surfData will be deleted in dtor

Todo Right now, we’re completely deleting the old data and then recopying the current data into a SurfData object. This was just the easiest way to arrive at a solution that would build and run. This function is frequently called from addPoint rebuild, however, and it’s not good to go through this whole process every time one more data point is added.

Reimplemented from Approximation.
References Dakota::abort_handler(), SharedApproxData::approxCLowerBnds, SharedApproxData::approxCUpperBnds, SharedApproxData::approxDILowerBnds, SharedApproxData::approxDIUpperBnds, SharedApproxData::approxDRLowerBnds, SharedApproxData::approxDRUpperBnds, Approximation::build(), SurfpackApproximation::factory, SharedSurfpackApproxData::merge_variable_arrays(), SurfpackApproximation::model, Approximation::sharedDataRep, SurfpackApproximation::surfData, and SurfpackApproximation::surrogates_to_surf_data().

const RealSymMatrix & hessian ( const Variables & vars ) [protected], [virtual]
retrieve the approximate function Hessian for a given parameter vector x

Todo Make this acceptably efficient

Reimplemented from Approximation.
References Dakota::abort_handler(), Approximation::approxHessian, SharedApproxData::approxType, Variables::cv(), SurfpackApproximation::model, and Approximation::sharedDataRep.
Referenced by SurfpackApproximation::add_anchor_to_surfdata().

const RealSymMatrix & hessian ( const RealVector & c_vars ) [protected], [virtual]
retrieve the approximate function Hessian for a given parameter vector x

Todo Make this acceptably efficient

Reimplemented from Approximation.
References Dakota::abort_handler(), Approximation::approxHessian, SharedApproxData::approxType, SurfpackApproximation::model, and Approximation::sharedDataRep.
SurfData * surrogates_to_surf_data( ) [private]

copy from SurrogateData to SurfPoint/SurfData

Copy the data stored in Dakota-style SurrogateData into Surfpack-style SurfPoint and SurfData objects.
References SurfpackApproximation::add_anchor_to_surfdata(), SharedSurfpackApproxData::add_sd_to_surfdata(), Approximation::approxData, SharedApproxData::buildDataOrder, SurfpackApproximation::factory, SharedApproxData::outputLevel, and Approximation::sharedDataRep.
Referenced by SurfpackApproximation::build().

void add_anchor_to_surfdata( SurfData & surf_data ) [private]

set the anchor point (including gradient and hessian if present) into surf_data

If there is an anchor point, add an equality constraint for its response value. Also add constraints for gradient and hessian, if applicable.
References Dakota::abort_handler(), Approximation::approxData, Dakota::copy_data(), SharedSurfpackApproxData::copy_matrix(), SurfpackApproximation::gradient(), SurfpackApproximation::hessian(), SharedApproxData::outputLevel, SharedSurfpackApproxData::svd_to_realarray(), and Approximation::sharedDataRep.
Referenced by SurfpackApproximation::surrogates_to_surf_data().
The documentation for this class was generated from the following files:

- SurfpackApproximation.hpp
- SurfpackApproximation.cpp

13.194 SurrBasedGlobalMinimizer Class Reference

The global surrogate-based minimizer which sequentially minimizes and updates a global surrogate model without trust region controls.

Inheritance diagram for SurrBasedGlobalMinimizer:

```
    Iterator
     |
    Minimizer
     |
SurrBasedMinimizer
     |
SurrBasedGlobalMinimizer
```

Public Member Functions

- SurrBasedGlobalMinimizer (ProblemDescDB &problem_db, Model &model)
  
  constructor
- ~SurrBasedGlobalMinimizer()
  
  destructor
Protected Member Functions

- void core_run ()
  Performs global surrogate-based optimization by repeatedly optimizing on and improving surrogates of the response functions.
- bool returns_multiple_points () const
  Global surrogate-based methods can return multiple points.

Private Attributes

- bool replacePoints
  flag for replacing the previous iteration’s point additions, rather than continuing to append, during construction of the next surrogate

Additional Inherited Members

13.194.1 Detailed Description

The global surrogate-based minimizer which sequentially minimizes and updates a global surrogate model without trust region controls.

This method uses a SurrogateModel to perform minimization (optimization or nonlinear least squares) through a set of iterations. At each iteration, a surrogate is built, the surrogate is minimized, and the optimal points from the surrogate are then evaluated with the "true" function, to generate new points upon which the surrogate for the next iteration is built.

The documentation for this class was generated from the following files:

- SurrBasedGlobalMinimizer.hpp
- SurrBasedGlobalMinimizer.cpp

13.195 SurrBasedLocalMinimizer Class Reference

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

Inheritance diagram for SurrBasedLocalMinimizer:

```
Iterator
  |
  v
Minimizer
  |
  v
SurrBasedMinimizer
  |
  v
SurrBasedLocalMinimizer
  |
  v
DataFitSurrBasedLocalMinimizer
  |
  v
HierarchSurrBasedLocalMinimizer
```
CHAPTER 13. CLASS DOCUMENTATION

Public Member Functions

- **SurrBasedLocalMinimizer** (ProblemDescDB &problem_db, Model &model)
  constructor

- ∼SurrBasedLocalMinimizer ()
  destructor

Protected Member Functions

- void **pre_run** ()
  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

- void **core_run** ()
  Performs local surrogate-based minimization by minimizing local, global, or hierarchical surrogates over a series of trust regions.

- void **post_run** (std::ostream &s)
  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

- void **reset** ()
  restore initial state for repeated sub-iterator executions

- virtual SurrBasedLevelData & **trust_region** ()=0
  return the active SurrBasedLevelData instance

- virtual void **update_trust_region** ()=0
  update the trust region bounds, strictly contained within global bounds

- virtual void **build** ()=0
  build the approximation over the current trust region

- virtual void **minimize** ()
  solve the approximate subproblem

- virtual void **verify** ()=0
  verify the approximate iterate and update the trust region for the next approximate optimization cycle

- virtual unsigned short **converged** ()=0
  return the convergence code for the truth level of the trust region hierarchy

- void **initialize_sub_model** ()
  construct and initialize approxSubProbModel

- void **initialize_sub_minimizer** ()
  construct and initialize approxSubProbMinimizer

- void **initialize_multipliers** ()
  initialize lagrangeMult and augLagrangeMult

- void **reset_penalties** ()
  reset all penalty parameters to their initial values

- void **reset_multipliers** ()
  reset Lagrange multipliers to initial values for cases where they are accumulated instead of computed directly

- void **update_trust_region_data** (SurrBasedLevelData &tr_data, const RealVector &parent_l_bnds, const RealVector &parent_u_bnds)
  update the trust region bounds, strictly contained within global bounds
• void update_approx_sub_problem (SurrBasedLevelData &tr_data)
  update variables and bounds within approxSubProbModel
• void compute_trust_region_ratio (SurrBasedLevelData &tr_data, bool check_interior=false)
  compute trust region ratio (for SBLM iterate acceptance and trust region resizing) and check for soft convergence (diminishing returns)
• void hard_convergence_check (SurrBasedLevelData &tr_data, const RealVector &lower_bnds, const RealVector &upper_bnds)
  check for hard convergence (norm of projected gradient of merit function < tolerance)
• void print_convergence_code (std::ostream &s, unsigned short code)
  print out the state corresponding to the code returned by converged()
• void update_penalty (const RealVector &fns_center_truth, const RealVector &fns_star_truth)
  initialize and update the penaltyParameter
• bool find_approx_response (const Variables &search_vars, Response &search_resp)
  locate an approximate response with the data_pairs cache
• bool find_truth_response (const Variables &search_vars, Response &search_resp)
  locate a truth response with the data_pairs cache
• bool find_response (const Variables &search_vars, Response &search_resp, const String &search_id, short set_request)
  locate a response with the data_pairs cache
• void relax_constraints (SurrBasedLevelData &tr_data)
  relax constraints by updating bounds when current iterate is infeasible

Static Protected Member Functions

• static void approx_subprob_objective_eval (const Variables &surrogate_vars, const Variables &recast_vars, const Response &surrogate_response, Response &recast_response)
  static function used to define the approximate subproblem objective.
• static void approx_subprob_constraint_eval (const Variables &surrogate_vars, const Variables &recast_vars, const Response &surrogate_response, Response &recast_response)
  static function used to define the approximate subproblem constraints.
• static void hom_objective_eval (int &mode, int &n, double *tau_and_x, double &f, double *grad_f, int &)
  static function used by NPSOL as the objective function in the homotopy constraint relaxation formulation.
• static void hom_constraint_eval (int &mode, int &ncnln, int &n, int &nrowj, int *needc, double *tau_and_x, double *c, double *cjac, int &nstate)
  static function used by NPSOL as the constraint function in the homotopy constraint relaxation formulation.

Protected Attributes

• Model approxSubProbModel
  the approximate sub-problem formulation solved on each approximate minimization cycle: may be a shallow copy of iteratedModel, or may involve a RecastModel recursion applied to iteratedModel
• short approxSubProbObj
  type of approximate subproblem objective: ORIGINAL_OBJ, LAGRANGIAN_OBJ, or AUGMENTED_LAGRANGIAN_OBJ
• short approxSubProbCon
type of approximate subproblem constraints: NO_CON, LINEARIZED_CON, or ORIGINAL_CON

- bool recastSubProb
  flag to indicate when approxSubProbModel involves a RecastModel recursion

- short meritFnType
  type of merit function used in trust region ratio logic: PENALTY_MERIT, ADAPTIVE_PENALTY_MERIT, LAGRANGIAN_MERIT, or AUGMENTED_LAGRANGIAN_MERIT

- short acceptLogic
  type of iterate acceptance test logic: FILTER or TR_RATIO

- short trConstraintRelax
  type of trust region constraint relaxation for infeasible starting points: NO_RELAX or HOMOTOPY

- int minimizeCycles
  counter for number of minimization cycles that have accumulated prior to convergence at the minimizeIndex level (used for ramping penalties)

- int penaltyIterOffset
  iteration offset used to update the scaling of the penalty parameter for adaptive_penalty merit functions

- RealVector origTrustRegionFactor
  original user specification for trust region initial size

- Real minTrustRegionFactor
  a soft convergence control: stop SBLM when the trust region factor is reduced below the value of minTrustRegionFactor

- Real trRatioContractValue
  trust region ratio min value: contract tr if ratio below this value

- Real trRatioExpandValue
  trust region ratio sufficient value: expand tr if ratio above this value

- Real gammaContract
  trust region contraction factor

- Real gammaExpand
  trust region expansion factor

- unsigned short softConvLimit
  convergence control limiting the number of consecutive iterations that fail to achieve sufficient decrease. If exceeded by softConvCount, stop.

- short truthSetRequest
  derivative order of truth data used within the SBLM process

- short approxSetRequest
  derivative order of surrogate data used within the SBLM process

- short correctionType
  flags the use of surrogate correction techniques at the center of each trust region

- RealVector initialPoint
  starting point prior to sequence of SBLM iterations

- RealVector globalLowerBnds
  Global lower bounds.

- RealVector globalUpperBnds
  Global Upper bounds.

- RealVector nonlinIneqLowerBndsSlack
individual violations of nonlinear inequality constraint lower bounds

- RealVector `nonlinIneqUpperBndsSlack`

individual violations of nonlinear inequality constraint upper bounds

- RealVector `nonlinEqTargetsSlack`

individual violations of nonlinear equality constraint targets

- Real `tau`

constraint relaxation parameter

- Real `alpha`

constraint relaxation parameter backoff parameter (multiplier)

Static Protected Attributes

- static `SurrBasedLocalMinimizer * sblmInstance`

pointer to SBLM instance used in static member functions

Additional Inherited Members

13.195.1 Detailed Description

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

This minimizer uses a `SurrogateModel` to perform minimization based on local, global, or hierarchical surrogates. It achieves provable convergence through the use of a sequence of trust regions and the application of surrogate corrections at the trust region centers.

13.195.2 Member Function Documentation

`surrBasedLocalMinimizer::pre_run( ) [protected], [virtual]`

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s `pre_run()`, if implemented, typically before performing its own implementation steps.

Reimplemented from `Iterator`.

References `Model::continuous_lower_bounds()`, `Model::continuous_upper_bounds()`, `Model::continuous_variables()`, `SurrBasedLocalMinimizer::converged()`, `Dakota::copy_data()`, `SurrBasedLocalMinimizer::globalLowerBnds`, `SurrBasedLocalMinimizer::globalUpperBnds`, `SurrBasedLocalMinimizer::initialPoint`, `Iterator::iteratedModel`, and `SurrBasedLocalMinimizer::reset()`.

Referenced by `HierarchSurrBasedLocalMinimizer::pre_run()`, and `DataFitSurrBasedLocalMinimizer::pre_run()`.

`surrBasedLocalMinimizer::core_run( ) [protected], [virtual]`

Performs local surrogate-based minimization by minimizing local, global, or hierarchical surrogates over a series of trust regions.

Trust region-based strategy to perform surrogate-based optimization in subregions (trust regions) of the parameter space. The minimizer operates on approximations in lieu of the more expensive simulation-based response functions. The size of the trust region is adapted according to the agreement between the approximations and the true response functions.

Reimplemented from `Iterator`.
References SurrBasedLocalMinimizer::build(), SurrBasedLocalMinimizer::converged(), SurrBasedLocalMinimizer::minimize(), SurrBasedLocalMinimizer::sblmInstance, SurrBasedLocalMinimizer::update_trust_region(), and SurrBasedLocalMinimizer::verify().

void post_run ( std::ostream & s ) [protected], [virtual]
post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent’s post_run(), typically after performing its own implementation steps.
Reimplemented from Minimizer.
References SurrBasedLocalMinimizer::converged(), SurrBasedMinimizer::globalIterCount, Minimizer::post_run(), and SurrBasedLocalMinimizer::print_convergence_code().
Referenced by HierarchSurrBasedLocalMinimizer::post_run(), and DataFitSurrBasedLocalMinimizer::post_run().

void compute_trust_region_ratio ( SurrBasedLevelData & tr_data, bool check_interior = false ) [protected]
compute trust region ratio (for SBLM iterate acceptance and trust region resizing) and check for soft convergence (diminishing returns)
Assess acceptance of SBLM iterate (trust region ratio or filter) and compute soft convergence metrics (number of consecutive failures, min trust region size, etc.) to assess whether the convergence rate has decreased to a point where the process should be terminated (diminishing returns).
References SurrBasedLocalMinimizer::acceptLogic, SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::augmented_lagrangian_merit(), SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, Iterator::convergenceTol, SurrBasedMinimizer::etaSequence, Response::function_values(), SurrBasedLocalMinimizer::gammaContract, SurrBasedLocalMinimizer::gammaExpand, SurrBasedMinimizer::initialize_filter(), Response::is_null(), Iterator::iteratedModel, SurrBasedMinimizer::lagrangian_merit(), SurrBasedLocalMinimizer::meritFnType, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, Iterator::outputLevel, SurrBasedMinimizer::penalty_merit(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Response::reset(), SurrBasedLocalMinimizer::trRatioContractValue, SurrBasedLocalMinimizer::trRatioExpandValue, SurrBasedMinimizer::update_augmented_lagrange_multipliers(), SurrBasedMinimizer::update_filter(), and SurrBasedLocalMinimizer::update_penalty().
Referenced by DataFitSurrBasedLocalMinimizer::verify(), and HierarchSurrBasedLocalMinimizer::verify().

void hard_convergence_check ( SurrBasedLevelData & tr_data, const RealVector & lower_bnds, const RealVector & upper_bnds ) [protected]
check for hard convergence (norm of projected gradient of merit function < tolerance)
The hard convergence check computes the gradient of the merit function at the trust region center, performs a projection for active bound constraints (removing any gradient component directed into an active bound), and signals convergence if the 2-norm of this projected gradient is less than convergenceTol.
References SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, Iterator::convergenceTol, Response::function_gradients(), Response::function_values(), Iterator::iteratedModel, SurrBasedMinimizer::lagrangian_gradient(), SurrBasedLocalMinimizer::meritFnType, SurrBasedLocalMinimizer::minimizeCycles, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, SurrBasedMinimizer::update_filter(), and SurrBasedLocalMinimizer::update_penalty().

void update_penalty ( const RealVector & fns_center_truth, const RealVector & fns_star_truth )  

initialize and update the penaltyParameter

Scaling of the penalty value is important to avoid rejecting SBLM iterates which must increase the objective to achieve a reduction in constraint violation. In the basic penalty case, the penalty is ramped exponentially based on the iteration counter. In the adaptive case, the ratio of relative change between center and star points for the objective and constraint violation values is used to rescale penalty values.

References SurrBasedMinimizer::alphaEta, SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, SurrBasedMinimizer::eta, SurrBasedMinimizer::etaSequence, Iterator::iteratedModel, SurrBasedLocalMinimizer::meritFnType, SurrBasedLocalMinimizer::penaltyIterOffset, SurrBasedMinimizer::penalty_Parameter, Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio().

void approx_subprob_objective_eval ( const Variables & surrogate_vars, const Variables & recast_vars, const Response & surrogate_response, Response & recast_response )  [static], [protected]

static function used to define the approximate subproblem objective.

Objective functions evaluator for solution of approximate subproblem using a RecastModel.

References Response::active_set_request_vector(), SurrBasedLocalMinimizer::approxSubProbCon, SurrBasedLocalMinimizer::approxSubProbModel, SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::augmented_lagrangian_gradient(), SurrBasedMinimizer::augmented_lagrangian_hessian(), SurrBasedMinimizer::augmented_lagrangian_merit(), Response::function_gradient(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian(), Response::function_hessians(), Response::function_value(), Response::function_values(), Iterator::iteratedModel, SurrBasedMinimizer::lagrangian_gradient(), SurrBasedMinimizer::lagrangian_hessian(), SurrBasedMinimizer::lagrangian_merit(), Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Minimizer::numUserPrimaryFns, Minimizer::objective(), Minimizer::objective_gradient(), Minimizer::objective_hessian(), SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinEqLowerBnds, SurrBasedMinimizer::origNonlinEqUpperBnds, Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), and SurrBasedLocalMinimizer::sblmInstance.

Referenced by SurrBasedLocalMinimizer::initialize_sub_model().

void approx_subprob_constraint_eval ( const Variables & surrogate_vars, const Variables & recast_vars, const Response & surrogate_response, Response & recast_response )  [static], [protected]

static function used to define the approximate subproblem constraints.

Constraint functions evaluator for solution of approximate subproblem using a RecastModel.

References Response::active_set_derivative_vector(), Response::active_set_request_vector(), SurrBasedLocalMinimizer::approxSubProbCon, SurrBasedLocalMinimizer::approxSubProbObj, Variables::continuous_variables(), Response::function_gradient(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian(), Response::function_hessian_view(), Response::function_value(), Response::function_values(), Minimizer::numUserPrimaryFns, SurrBasedLocalMinimizer::sblmInstance, and SurrBasedLocalMinimizer::trust_region().

Referenced by SurrBasedLocalMinimizer::initialize_sub_model().
void hom_objective_eval ( int & mode, int & n, double * tau_and_x, double & f, double * grad_f, int & ) [static], [protected]

static function used by NPSOL as the objective function in the homotopy constraint relaxation formulation.

NPSOL objective functions evaluator for solution of homotopy constraint relaxation parameter optimization. This constrained optimization problem performs the update of the tau parameter in the homotopy heuristic approach used to relax the constraints in the original problem.

Referenced by SurrBasedLocalMinimizer::relax_constraints().

void hom_constraint_eval ( int & mode, int & ncnln, int & n, int & nrowj, int * needc, double * tau_and_x, double * c, double * cjac, int & nstate ) [static], [protected]

static function used by NPSOL as the constraint function in the homotopy constraint relaxation formulation.

NPSOL constraint functions evaluator for solution of homotopy constraint relaxation parameter optimization. This constrained optimization problem performs the update of the tau parameter in the homotopy heuristic approach used to relax the constraints in the original problem.

References Response::active_set(), SurrBasedLocalMinimizer::approxSubProbModel, Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_values(), SurrBasedLocalMinimizer::nonlinEqTargetsSlack, SurrBasedLocalMinimizer::nonlinIneqLowerBndsSlack, SurrBasedLocalMinimizer::nonlinIneqUpperBndsSlack, Model::num_functions(), Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, ActiveSet::request_vector(), SurrBasedLocalMinimizer::sblmInstance, and SurrBasedLocalMinimizer::tau.

Referenced by SurrBasedLocalMinimizer::relax_constraints().

The documentation for this class was generated from the following files:

- SurrBasedLocalMinimizer.hpp
- SurrBasedLocalMinimizer.cpp

13.196  SurrBasedMinimizer Class Reference

Base class for local/global surrogate-based optimization/least squares.

Inheritance diagram for SurrBasedMinimizer:

```
Iterator
|
| Minimizer
| |
SurrBasedMinimizer
 |
| EffGlobalMinimizer
| SurrBasedGlobalMinimizer
| SurrBasedLocalMinimizer
|
| DataFitSurrBasedLocalMinimizer
| HierarchSurrBasedLocalMinimizer
```

Protected Member Functions

- **SurrBasedMinimizer (ProblemDescDB &problem_db, Model &model)**
  
  *constructor*

- **~SurrBasedMinimizer ()**
  
  *destructor*
• void derived_init_communicators (ParLevIter pl_iter)
  derived class contributions to initializing the communicators associated with this Iterator instance

• void derived_set_communicators (ParLevIter pl_iter)
  derived class contributions to setting the communicators associated with this Iterator instance

• void derived_free_communicators (ParLevIter pl_iter)
  derived class contributions to freeing the communicators associated with this Iterator instance

• void initialize_graphics (int iterator_server_id=1)
  initialize graphics customized for surrogate-based iteration

• void print_results (std::ostream &s)

• void update_lagrange_multipliers (const RealVector &fn_vals, const RealMatrix &fn_grads)
  initialize and update Lagrange multipliers for basic Lagrangian

• void update_augmented_lagrange_multipliers (const RealVector &fn_vals)
  initialize and update the Lagrange multipliers for augmented Lagrangian

• void initialize_filter (SurrBasedLevelData &tr_data, const RealVector &fn_vals)
  (re-)initialize filter from a set of function values

• bool update_filter (SurrBasedLevelData &tr_data, const RealVector &fn_vals)
  update filter using a new set of function values

• Real lagrangian_merit (const RealVector &fn_vals, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts)
  compute a Lagrangian function from a set of function values

• void lagrangian_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealVector &lag_grad)
  compute the gradient of the Lagrangian function

• void lagrangian_hessian (const RealVector &fn_vals, const RealMatrix &fn_grads, const RealSymMatrixArray &fn_hessians, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealSymMatrix &lag_hess)
  compute the Hessian of the Lagrangian function

• Real augmented_lagrangian_merit (const RealVector &fn_vals, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts)
  compute an augmented Lagrangian function from a set of function values

• void augmented_lagrangian_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealVector &alag_grad)
  compute the gradient of the augmented Lagrangian function

• void augmented_lagrangian_hessian (const RealVector &fn_vals, const RealMatrix &fn_grads, const RealSymMatrixArray &fn_hessians, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealSymMatrix &alag_hess)
  compute the Hessian of the augmented Lagrangian function

• Real penalty_merit (const RealVector &fn_vals, const BoolDeque &sense, const RealVector &primary_wts)
  compute a penalty function from a set of function values
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- void penalty_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &sense, const RealVector &primary_wts, RealVector &pen_grad)
  compute the gradient of the penalty function
- Real constraint_violation (const RealVector &fn_vals, const Real &constraint_tol)
  compute the constraint violation from a set of function values

Protected Attributes

- Iterator approxSubProbMinimizer
  the minimizer used on the surrogate model to solve the approximate subproblem on each surrogate-based iteration
- size_t globalIterCount
  global iteration counter corresponding to number of surrogate-based minimizations
- RealVector lagrangeMult
  Lagrange multipliers for basic Lagrangian calculations.
- RealVector augLagrangeMult
  Lagrange multipliers for augmented Lagrangian calculations.
- Real penaltyParameter
  the penalization factor for violated constraints used in quadratic penalty calculations; increased in update_penalty()
- RealVector origNonlinIneqLowerBnds
  original nonlinear inequality constraint lower bounds (no relaxation)
- RealVector origNonlinIneqUpperBnds
  original nonlinear inequality constraint upper bounds (no relaxation)
- RealVector origNonlinEqTargets
  original nonlinear equality constraint targets (no relaxation)
- Real eta
  constant used in etaSequence updates
- Real alphaEta
  power for etaSequence updates when updating penalty
- Real betaEta
  power for etaSequence updates when updating multipliers
- Real etaSequence
  decreasing sequence of allowable constraint violation used in augmented Lagrangian updates (refer to Conn, Gould, and Toint, section 14.4)
- size_t miPLIndex
  index for the active ParallelLevel within ParallelConfiguration::miPLIters

Additional Inherited Members

13.196.1 Detailed Description

Base class for local/global surrogate-based optimization/least squares.
These minimizers use a SurrogateModel to perform optimization based either on local trust region methods or global updating methods.
13.196.2 Member Function Documentation

void print_results ( std::ostream & s ) [protected], [virtual]

Redefines default iterator results printing to include optimization results (objective functions and constraints).

Reimplemented from Iterator.

References Dakota::abort_handler(), Iterator::activeSet, Minimizer::archive_allocate_best(), Minimizer::archive_best(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Dakota::data_pairs, Model::interface_id(), Iterator::iteratedModel, Dakota::lookup_by_val(), Iterator::methodName, Minimizer::numFunctions, Minimizer::numUserPrimaryFns, Minimizer::optimizationFlag, ActiveSet::request_values(), and Model::truth_model().

void update_lagrange_multipliers ( const RealVector & fn_vals, const RealMatrix & fn_grads ) [protected]

initialize and update Lagrange multipliers for basic Lagrangian

For the Rockafellar augmented Lagrangian, simple Lagrange multiplier updates are available which do not require the active constraint gradients. For the basic Lagrangian, Lagrange multipliers are estimated through solution of a nonnegative linear least squares problem.

References Dakota::abort_handler(), Minimizer::bigRealBoundSize, Minimizer::constraintTol, Iterator::iteratedModel, SurrBasedMinimizer::lagrangeMult, Minimizer::numContinuousVars, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, Minimizer::objective_gradient(), SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by SurrBasedLocalMinimizer::hard_convergence_check().

void update_augmented_lagrange_multipliers ( const RealVector & fn_vals ) [protected]

initialize and update the Lagrange multipliers for augmented Lagrangian

For the Rockafellar augmented Lagrangian, simple Lagrange multiplier updates are available which do not require the active constraint gradients. For the basic Lagrangian, Lagrange multipliers are estimated through solution of a nonnegative linear least squares problem.

References SurrBasedMinimizer::augLagrangeMult, SurrBasedMinimizer::betaEta, Minimizer::bigRealBoundSize, SurrBasedMinimizer::etaSequence, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, and SurrBasedMinimizer::penalty_Parameter.

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio(), SurrBasedLocalMinimizer::hard_convergence_check(), and EffGlobalMinimizer::minimize_surrogates_on_model().

bool update_filter ( SurrBasedLevelData & tr_data, const RealVector & fn_vals ) [protected]

update filter using a new set of function values

Update the paretoFilter with fn_vals if new iterate is non-dominated.

References SurrBasedMinimizer::constraint_violation(), Iterator::iteratedModel, Minimizer::numNonlinearConstraints, Minimizer::objective(), Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio().
compute a Lagrangian function from a set of function values

The Lagrangian function computation sums the objective function and the Lagrange multiplier terms for inequality/equality constraints. This implementation follows the convention in Vanderplaats with \( g < 0 \) and \( h = 0 \). The bounds/targets passed in may reflect the original constraints or the relaxed constraints.

References Minimizer::bigRealBoundSize, Minimizer::constraintTol, SurrBasedMinimizer::lagrangeMult, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, and Minimizer::objective().

Referenced by SurrBasedLocalMinimizer::approx_subprob_objective_eval(), and SurrBasedLocalMinimizer::compute_trust_region_ratio().

compute an augmented Lagrangian function from a set of function values

The Rockafellar augmented Lagrangian function sums the objective function, Lagrange multiplier terms for inequality/equality constraints, and quadratic penalty terms for inequality/equality constraints. This implementation follows the convention in Vanderplaats with \( g < 0 \) and \( h = 0 \). The bounds/targets passed in may reflect the original constraints or the relaxed constraints.

References SurrBasedMinimizer::augLagrangeMult, Minimizer::bigRealBoundSize, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, Minimizer::objective(), and SurrBasedMinimizer::penaltyParameter.

Referenced by SurrBasedLocalMinimizer::approx_subprob_objective_eval(), SurrBasedLocalMinimizer::compute_trust_region_ratio(), EffGlobalMinimizer::get_best_sample(), and EffGlobalMinimizer::minimize_surrogates_on_model().

compute a penalty function from a set of function values

The penalty function computation applies a quadratic penalty to any constraint violations and adds this to the objective function(s) \( p = f + r_p \cdot cv \).

References SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, Minimizer::objective(), and SurrBasedMinimizer::penaltyParameter.

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio().

compute the constraint violation from a set of function values

Compute the quadratic constraint violation defined as \( cv = g^+ \cdot h^+ \). This implementation supports equality constraints and 2-sided inequalities. The constraint_tol allows for a small constraint infeasibility (used for penalty methods, but not Lagrangian methods).

References Minimizer::bigRealBoundSize, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, and SurrBasedMinimizer::origNonlinIneqUpperBnds.
Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio(), SurrBasedLocalMinimizer::hard_convergence_check(), SurrBasedMinimizer::initialize_filter(), EffGlobalMinimizer::minimize_surrogates_on_model(), SurrBasedMinimizer::penalty_merit(), SurrBasedLocalMinimizer::relax_constraints(), SurrBasedMinimizer::update_filter(), and SurrBasedLocalMinimizer::update_penalty().

The documentation for this class was generated from the following files:

- SurrBasedMinimizer.hpp
- SurrBasedMinimizer.cpp

### 13.197 SurrogateModel Class Reference

Base class for surrogate models (DataFitSurrModel and HierarchSurrModel).

Inheritance diagram for SurrogateModel:

```
Model
   SurrogateModel
   DataFitSurrModel
   HierarchSurrModel
```

#### Protected Member Functions

- **SurrogateModel (ProblemDescDB &problem_db)**  
  constructor
- **SurrogateModel (ProblemDescDB &problem_db, ParallelLibrary &parallel_lib, const SharedVariablesData &svd, const SharedResponseData &srd, const ActiveSet &set, short corr_type, short output_level)**  
  alternate constructor
- **~SurrogateModel ()**  
  destructor
- **bool initialize_mapping (ParLevLIter pl_iter)**  
  initialize model mapping, returns true if the variables size has changed
- **bool finalize_mapping ()**  
  finalize model mapping, returns true if the variables size has changed
- **bool mapping_initialized () const**  
  return mappingInitialized
- **Model & subordinate_model ()**  
  return truth_model()
- **short surrogate_response_mode () const**  
  return responseMode
- **int derived_evaluation_id () const**  
  return the current evaluation id for this Model
- **size_t mi_parallel_level_index () const**  
  return miPLIndex
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- **void check_submodel_compatibility** (const Model &sub_model)
  
  verify compatibility between SurrogateModel attributes and attributes of the submodel (DataFitSurrModel::actualModel or HierarchSurrModel::highFidelityModel)

- **void check_key** (int key1, int key2) const
  
  check for consistency in response map keys

- **bool force_rebuild ()**
  
  evaluate whether a rebuild of the approximation should be forced based on changes in the inactive data

- **void asv_mapping** (const ShortArray &orig_asv, ShortArray &actual_asv, ShortArray &approx_asv, bool build_flag)
  
  distributes the incoming orig_asv among actual_asv and approx_asv

- **void asv_mapping** (const ShortArray &actual_asv, const ShortArray &approx_asv, ShortArray &combined_asv)
  
  reconstitutes a combined_asv from actual_asv and approx_asv

- **void response_mapping** (const Response &actual_response, const Response &approx_response, Response &combined_response)
  
  overlays actual_response and approx_response to update combined_response

- **void aggregate_response** (const Response &hf_resp, const Response &lf_resp, Response &agg_resp)
  
  aggregate LF and HF response to create a new response with 2x size

### Protected Attributes

- **IntSet surrogateFnIndices**
  
  for mixed response sets, this array specifies the response function subset that is approximated

- **short responseMode**
  
  an enumeration that controls the response calculation mode in \{DataFit,Hierarch\}SurrModel approximate response computations

- **short corrType**
  
  type of correction: additive, multiplicative, or combined

- **IntlIntMap truthIdMap**
  
  map from actualModel/highFidelityModel evaluation ids to DataFitSurrModel/HierarchSurrModel ids

- **IntlIntMap surrIdMap**
  
  map from approxInterface/lowFidelityModel evaluation ids to DataFitSurrModel/HierarchSurrModel ids

- **int surrModelEvalCntr**
  
  counter for calls to derived_evaluate()/derived_evaluate_nowait(); used to key response maps from SurrogateModels

- **IntlResponseMap surrResponseMap**
  
  map of surrogate responses returned by derived_synchronize() and derived_synchronize_nowait()

- **IntlResponseMap cachedApproxRespMap**
  
  map of approximate responses retrieved in derived_synchronize_nowait() that could not be returned since corresponding truth model response portions were still pending.

- **IntlVariablesMap rawVarsMap**
  
  map of raw continuous variables used by apply_correction(). Model::varsList cannot be used for this purpose since it does not contain lower level variables sets from finite differencing.

- **size_t approxBuilds**
  
  number of calls to build_approximation()

- **size_t miPLIndex**
the index of the active metaiterator-iterator parallelism level (corresponding to ParallelConfiguration::miPLIters) used at runtime

- **RealVector referenceCLBnds**
  stores a reference copy of active continuous lower bounds when the approximation is built; used to detect when a rebuild is required.

- **RealVector referenceCUBnds**
  stores a reference copy of active continuous upper bounds when the approximation is built; used to detect when a rebuild is required.

- **IntVector referenceDILBnds**
  stores a reference copy of active discrete int lower bounds when the approximation is built; used to detect when a rebuild is required.

- **IntVector referenceDIUBnds**
  stores a reference copy of active discrete int upper bounds when the approximation is built; used to detect when a rebuild is required.

- **RealVector referenceDRLBnds**
  stores a reference copy of active discrete real lower bounds when the approximation is built; used to detect when a rebuild is required.

- **RealVector referenceDRUBnds**
  stores a reference copy of active discrete real upper bounds when the approximation is built; used to detect when a rebuild is required.

- **RealVector referenceICVars**
  stores a reference copy of the inactive continuous variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.

- **IntVector referenceIDIVars**
  stores a reference copy of the inactive discrete int variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.

- **StringMultiArray referenceIDSVars**
  stores a reference copy of the inactive discrete string variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.

- **RealVector referenceIDRVars**
  stores a reference copy of the inactive discrete real variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.

**Private Attributes**

- **Variables truthModelVars**
  copy of the truth model variables object used to simplify conversion among differing variable views in force_rebuild()

- **Constraints truthModelCons**
  copy of the truth model constraints object used to simplify conversion among differing variable views in force_rebuild()

- **bool mappingInitialized**
  track use of initialize_mapping() and finalize_mapping() due to potential redundancy between IteratorScheduler::run_iterator() and {Analyzer,Minimizer}::initialize_run()
Additional Inherited Members

13.197.1 Detailed Description

Base class for surrogate models (DataFitSurrModel and HierarchSurrModel).

The SurrogateModel class provides common functions to derived classes for computing and applying corrections to approximations.

13.197.2 Member Function Documentation

int derivated_evaluation_id ( ) const [inline], [protected], [virtual]

return the current evaluation id for this Model

return the SurrogateModel evaluation id counter. Due to possibly intermittent use of lower level components, this is not the same as approxInterface, actualModel, or orderedModels evaluation counts, which requires a consistent evaluation rekeying process.

Reimplemented from Model.

References SurrogateModel::surrModelEvalCntr.

bool force_rebuild ( ) [protected], [virtual]

evaluate whether a rebuild of the approximation should be forced based on changes in the inactive data

This function forces a rebuild of the approximation according to the sub-model variables view, the approximation type, and whether the active approximation bounds or inactive variable values have changed since the last approximation build.

Reimplemented from Model.

References Constraints::all_continuous_lower_bounds(), Constraints::all_continuous_upper_bounds(), Variables::all_continuous_variables(), Constraints::all_discrete_int_lower_bounds(), Constraints::all_discrete_int_upper_bounds(), Variables::all_discrete_int_variables(), Constraints::all_discrete_real_lower_bounds(), Constraints::all_discrete_real_upper_bounds(), Variables::all_discrete_real_variables(), Variables::all_discrete_string_variables(), Constraints::continuous_lower_bounds(), Model::continuous_lower_bounds(), Constraints::continuous_upper_bounds(), Model::continuous_upper_bounds(), Variables::continuous_variables(), Constraints::copy(), Variables::copy(), Model::current_variables(), Model::current_variables(), Constraints::discrete_int_lower_bounds(), Model::discrete_int_lower_bounds(), Constraints::discrete_int_upper_bounds(), Model::discrete_int_upper_bounds(), Variables::discrete_int_variables(), Constraints::discrete_real_lower_bounds(), Model::discrete_real_lower_bounds(), Constraints::discrete_real_upper_bounds(), Model::discrete_real_upper_bounds(), Variables::discrete_real_variables(), Variables::discrete_string_variables(), Variables::inactive_continuous_variables(), Variables::inactive_discrete_int_variables(), Variables::inactive_discrete_real_variables(), Variables::inactive_discrete_string_variables(), Constraints::is_null(), Variables::is_null(), Model::is_null(), Model::model_type(), SurrogateModel::referenceCLBnds, SurrogateModel::referenceCUBnds, SurrogateModel::referenceDIUBnds, SurrogateModel::referenceDRLBnds, SurrogateModel::referenceDRUBnds, SurrogateModel::referenceICVars, SurrogateModel::referenceIDIVars, SurrogateModel::referenceIDRVars, SurrogateModel::referenceIDSVars, Dakota::strbegins(), Model::subordinate_model(), Model::surrogateType, Model::truth_model(), SurrogateModel::truthModelCons, SurrogateModel::truthModelVars, Model::user_defined_constraints(), Model::userDefinedConstraints, and Variables::view().

Referenced by HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate_nowait(), and DataFitSurrModel::derived_evaluate_nowait().
13.197.3 Member Data Documentation

short responseMode [protected]

an enumeration that controls the response calculation mode in {DataFit,Hierarch}SurrModel approximate response computations

SurfBasedLocalMinimizer toggles this mode since compute_correction() does not back out old corrections.

Referenced by HierarchSurrModel::component_parallel_mode(), HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate_nowait(), DataFitSurrModel::derived_evaluate_nowait(), HierarchSurrModel::derived_set_communicators(), DataFitSurrModel::derived_synchronize(), DataFitSurrModel::derived_synchronize_approx(), HierarchSurrModel::derived_synchronize_combine(), HierarchSurrModel::derived_synchronize_combine_nowait(), DataFitSurrModel::derived_synchronize_nowait(), HierarchSurrModel::derived_synchronize_sequential(), HierarchSurrModel::resize_response(), HierarchSurrModel::serve_run(), SurrogateModel::surrogate_response_mode(), HierarchSurrModel::surrogate_response_mode(), DataFitSurrModel::surrogate_response_mode(), DataFitSurrModel::surrogate_response_mode(), and SurrogateModel::SurrogateModel().

size_t approxBuilds [protected]

number of calls to build_approximation()

used as a flag to automatically build the approximation if one of the derived evaluate functions is called prior to build_approximation().

Referenced by DataFitSurrModel::append_approximation(), DataFitSurrModel::approximation_coefficients(), HierarchSurrModel::build_approximation(), DataFitSurrModel::build_approximation(), HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate_nowait(), DataFitSurrModel::derived_evaluate_nowait(), HierarchSurrModel::init_model(), DataFitSurrModel::init_model(), DataFitSurrModel::pop_approximation(), DataFitSurrModel::update_approximation(), and DataFitSurrModel::update_from_model().

The documentation for this class was generated from the following files:

- SurrogateModel.hpp
- SurrogateModel.cpp

13.198 SysCallApplicInterface Class Reference

Derived application interface class which spawns simulation codes using system calls.

Inheritance diagram for SysCallApplicInterface:
Public Member Functions

- **SysCallApplicInterface** (const ProblemDescDB &problem_db)
  
  constructor

- **~SysCallApplicInterface** ()
  
  destructor

Protected Member Functions

- void wait_local_evaluations (PRPQueue &prp_queue)
- void test_local_evaluations (PRPQueue &prp_queue)
- int synchronous_local_analysis (int analysis_id)
- void init_communicators_checks (int max_eval_concurrency)
- void set_communicators_checks (int max_eval_concurrency)
- void map_bookkeeping (pid_t pid, int fn_eval_id)
  
  bookkeeping of process and evaluation ids for asynchronous maps

- pid_t create_evaluation_process (bool block_flag)
  
  Spawn the evaluation by managing the input filter, analysis drivers, and output filter. Called from derived_map() & derived_map_asynch().

Private Member Functions

- bool system_call_file_test (const bfs::path &root_file)
  
  detect completion of a function evaluation through existence of the necessary results file(s)

- void spawn_evaluation_to_shell (bool block_flag)
  
  spawn a complete function evaluation

- void spawn_input_filter_to_shell (bool block_flag)
  
  spawn the input filter portion of a function evaluation

- void spawn_analysis_to_shell (int analysis_id, bool block_flag)
  
  spawn a single analysis as part of a function evaluation

- void spawn_output_filter_to_shell (bool block_flag)
  
  spawn the output filter portion of a function evaluation

Private Attributes

- IntSet sysCallSet
  
  set of function evaluation id's for active asynchronous system call evaluations

- IntShortMap failCountMap
  
  map linking function evaluation id's to number of response read failures

Additional Inherited Members

13.198.1 Detailed Description

Derived application interface class which spawns simulation codes using system calls.

system() is part of the C API and can be used on both Windows and Unix systems.
13.198.2 Member Function Documentation

void \texttt{wait} ( PRPQueue & \texttt{prp\_queue}) \ [inline], \ [protected], \ [virtual]

Check for completion of active asynch jobs (tracked with sysCallSet). Wait for at least one completion and complete all jobs that have returned. This satisfies a "fairness" principle, in the sense that a completed job will always be processed (whereas accepting only a single completion could always accept the same completion - the case of very inexpensive fn. evals. - and starve some servers).

Reimplemented from ApplicationInterface.

References ApplicationInterface::completionSet, and SysCallApplicInterface::test\_local\_evaluations().

void \texttt{test\_local\_evaluations} ( PRPQueue & \texttt{prp\_queue}) \ [protected], \ [virtual]

Check for completion of active asynch jobs (tracked with sysCallSet). Make one pass through sysCallSet & complete all jobs that have returned.

Reimplemented from ApplicationInterface.

Reimplemented from Dakota::abort\_handler(), Response::active\_set(), ApplicationInterface::completionSet, SysCallApplicInterface::failCountMap, ProcessApplicInterface::fileNameMap, Interface::final\_eval\_id\_tag(), Dakota::lookup\_by\_eval\_id(), ApplicationInterface::manage\_failure(), ProcessApplicInterface::read\_results\_files(), SysCallApplicInterface::sysCallSet, and SysCallApplicInterface::sytem\_call\_file\_test().

Referenced by SysCallApplicInterface::wait\_local\_evaluations().

int \texttt{synchronous\_local\_analysis} ( int \texttt{analysis\_id}) \ [inline], \ [protected], \ [virtual]

This code provides the derived function used by ApplicationInterface::serve\_analyses\_synch().

Reimplemented from ApplicationInterface.

References SysCallApplicInterface::spawn\_analysis\_to\_shell().

void \texttt{init\_communicators\_checks} ( int \texttt{max\_eval\_concurrency}) \ [inline], \ [protected], \ [virtual]

No derived interface plug-ins, so perform construct-time checks. However, process init issues as warnings since some contexts (e.g., Hierarch\_Surr\_Model) initialize more configurations than will be used.

Reimplemented from ApplicationInterface.

References ApplicationInterface::check\_multiprocessor\_analysis().

void \texttt{set\_communicators\_checks} ( int \texttt{max\_eval\_concurrency}) \ [inline], \ [protected], \ [virtual]

Process run-time issues as hard errors.

Reimplemented from ApplicationInterface.

References Dakota::abort\_handler(), and ApplicationInterface::check\_multiprocessor\_analysis().

void \texttt{spawn\_evaluation\_to\_shell} ( bool \texttt{block\_flag}) \ [private]

spawn a complete function evaluation

Put the SysCallApplicInterface to the shell. This function is used when all portions of the function evaluation (i.e., all analysis drivers) are executed on the local processor.

References CommandShell::asynch\_flag(), ProcessApplicInterface::commandLine\_Args, ProcessApplicInterface::cur\_Workdir, Dakota::flush(), ProcessApplicInterface::iFilter\_Name, ProcessApplicInterface::multiple\_Params\_Files, ProcessApplicInterface::oFilter\_Name, ProcessApplicInterface::params\_FileName, ProcessApplicInterface::prepare\_process\_environment(), ProcessApplicInterface::program\_Names, ProcessApplicInterface::reset\_process\_environment(),
ProcessApplicInterface::resultsFileName, CommandShell::suppress_output_flag(), ApplicationInterface::suppressOutput, and ProcessApplicInterface::useWorkdir.
    Referenced by SysCallApplicInterface::create_evaluation_process().

```cpp
void spawn_input_filter_to_shell ( bool block_flag ) [private]
```

spawn the input filter portion of a function evaluation

Put the input filter to the shell. This function is used when multiple analysis drivers are spread between processors. No need to check for a Null input filter, as this is checked externally. Use of nonblocking shells is supported in this fn, although its use is currently prevented externally.

References CommandShell::asynch_flag(), ProcessApplicInterface::commandLineArgs, Dakota::flush(), ProcessApplicInterface::ifFilterName, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::prepare_process_environment(), ProcessApplicInterface::reset_process_environment(), ProcessApplicInterface::resultsFileName, CommandShell::suppress_output_flag(), and ApplicationInterface::suppressOutput.

Referenced by SysCallApplicInterface::create_evaluation_process().

```cpp
void spawn_analysis_to_shell ( int analysis_id, bool block_flag ) [private]
```

spawn a single analysis as part of a function evaluation

Put a single analysis to the shell. This function is used when multiple analysis drivers are spread between processors. Use of nonblocking shells is supported in this fn, although its use is currently prevented externally.

References CommandShell::asynch_flag(), ProcessApplicInterface::commandLineArgs, Dakota::flush(), ProcessApplicInterface::multipleParamsFiles, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::prepare_process_environment(), ProcessApplicInterface::programNames, ProcessApplicInterface::reset_process_environment(), ProcessApplicInterface::resultsFileName, CommandShell::suppress_output_flag(), and ApplicationInterface::suppressOutput.

Referenced by SysCallApplicInterface::create_evaluation_process(), SysCallApplicInterface::synchronous_local_analysis(), and GridApplicInterface::synchronous_local_analysis().

```cpp
void spawn_output_filter_to_shell ( bool block_flag ) [private]
```

spawn the output filter portion of a function evaluation

Put the output filter to the shell. This function is used when multiple analysis drivers are spread between processors. No need to check for a Null output filter, as this is checked externally. Use of nonblocking shells is supported in this fn, although its use is currently prevented externally.

References CommandShell::asynch_flag(), ProcessApplicInterface::commandLineArgs, Dakota::flush(), ProcessApplicInterface::oFilterName, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::prepare_process_environment(), ProcessApplicInterface::reset_process_environment(), ProcessApplicInterface::resultsFileName, CommandShell::suppress_output_flag(), and ApplicationInterface::suppressOutput.

Referenced by SysCallApplicInterface::create_evaluation_process().

The documentation for this class was generated from the following files:

- SysCallApplicInterface.hpp
- SysCallApplicInterface.cpp

### 13.199 TabularDataTruncated Class Reference

exception thrown when data read truncated

Inheritance diagram for TabularDataTruncated:
TabularDataTruncated

Public Member Functions

- **TabularDataTruncated**(const std::string &msg)

### 13.199.1 Detailed Description

Exception thrown when data read truncated
The documentation for this class was generated from the following file:
- dakota_global_defs.hpp

### 13.200 TabularReader Class Reference

Utility used in derived read_core to read values in tabular format.

Public Member Functions

- template<typename ArrayType>
  void **operator()**( std::istream &s, size_t start_index, size_t num_items, ArrayType &array_data, StringMultiArrayView label_array)

### 13.200.1 Detailed Description

Utility used in derived read_core to read values in tabular format.

### 13.200.2 Member Function Documentation

void **operator()**( std::istream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array) [inline]

The tabular reader doesn’t forward the label arrays
The documentation for this class was generated from the following file:
- DakotaVariables.hpp

### 13.201 TabularWriter Class Reference

Utility used in derived write_core to write values in tabular format.

Public Member Functions

- template<typename ArrayType>
  void **operator()**( std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array)
13.201.1 Detailed Description

Utility used in derived write_core to write values in tabular format.

13.201.2 Member Function Documentation

void operator() ( std::ostream & s, size_t start_index, size_t num_items, const ArrayType & array_data, StringMultiArrayConstView label_array ) [inline]

The tabular writer doesn’t forward the label arrays

The documentation for this class was generated from the following file:

- DakotaVariables.hpp

13.202 TANA3Approximation Class Reference

Derived approximation class for TANA-3 two-point exponential approximation (a multipoint approximation).

Inheritance diagram for TANA3Approximation:

```
Approximation
   |     
   v     
TANA3Approximation
```

Public Member Functions

- TANA3Approximation ()
  default constructor
- TANA3Approximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)
  standard constructor
- TANA3Approximation (const SharedApproxData &shared_data)
  alternate constructor
- ~TANA3Approximation ()
  destructor

Protected Member Functions

- int min_coefficients () const
  return the minimum number of samples (unknowns) required to build the derived class approximation type in num-Vars dimensions
- int num_constraints () const
  return the number of constraints to be enforced via an anchor point
- void build ()
  builds the approximation from scratch
- Real value (const Variables &vars)
retrieve the approximate function value for a given parameter vector

- const RealVector & gradient (const Variables & vars)

retrieve the approximate function gradient for a given parameter vector

- void clear_current ()

Private Member Functions

- void find_scaled_coefficients ()
  compute TANA coefficients based on scaled inputs

- void offset (const RealVector & x, RealVector & s)
  based on minX, apply offset scaling to x to define s

Private Attributes

- RealVector pExp
  vector of exponent values

- RealVector minX
  vector of minimum parameter values used in scaling

- RealVector scX1
  vector of scaled x1 values

- RealVector scX2
  vector of scaled x2 values

- Real H
  the scalar Hessian value in the TANA-3 approximation

Additional Inherited Members

13.202.1 Detailed Description

Derived approximation class for TANA-3 two-point exponential approximation (a multipoint approximation).

The TANA3Approximation class provides a multipoint approximation based on matching value and gradient data from two points (typically the current and previous iterates) in parameter space. It forms an exponential approximation in terms of intervening variables.

13.202.2 Member Function Documentation

void build ( ) [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References Dakota::abort_handler(), Approximation::approxData, Approximation::build(), TANA3Approximation::find_scaled_coefficients(), TANA3Approximation::minX, SharedApproxData::numVars, TANA3Approximation::pExp, and Approximation::sharedDataRep.
void clear_current() [inline], [protected], [virtual]

Redefine default implementation to support history mechanism.
Reimplemented from Approximation.
References Approximation::approxData.
The documentation for this class was generated from the following files:
  - TANA3Approximation.hpp
  - TANA3Approximation.cpp

### 13.203 TaylorApproximation Class Reference

Derived approximation class for first- or second-order Taylor series (a local approximation).
Inheritance diagram for TaylorApproximation:

```
Approximation

TaylorApproximation
```

#### Public Member Functions

- `TaylorApproximation()`
  *default constructor*
- `TaylorApproximation(ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)`
  *standard constructor*
- `TaylorApproximation(const SharedApproxData &shared_data)`
  *alternate constructor*
- `~TaylorApproximation()`
  *destructor*

#### Protected Member Functions

- `int min_coefficients()` const
  *return the minimum number of samples (unknowns) required to build the derived class approximation type in num-Vars dimensions*
- `void build()`
  *builds the approximation from scratch*
- `Real value(const Variables &vars)`
  *retrieve the approximate function value for a given parameter vector*
- `const RealVector & gradient(const Variables &vars)`
  *retrieve the approximate function gradient for a given parameter vector*
- `const RealSymMatrix & hessian(const Variables &vars)`
  *retrieve the approximate function Hessian for a given parameter vector*
Additional Inherited Members

13.203.1 Detailed Description

Derived approximation class for first- or second-order Taylor series (a local approximation).

The TaylorApproximation class provides a local approximation based on data from a single point in parameter space. It uses a zeroth-, first- or second-order Taylor series expansion: \( f(x) = f(x_c) \) for zeroth-order, plus \( \text{grad}(x - x_c)' (x - x_c) \) for first- and second-order, and plus \( (x - x_c)' \text{Hess}(x_c) (x - x_c) / 2 \) for second-order.

13.203.2 Member Function Documentation

void build() [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References Dakota::abort_handler(), Approximation::approxData, Approximation::build(), SharedApproxData::buildDataOrder, SharedApproxData::numVars, and Approximation::sharedDataRep.

The documentation for this class was generated from the following files:

- TaylorApproximation.hpp
- TaylorApproximation.cpp

13.204 TestDriverInterface Class Reference

Inheritance diagram for TestDriverInterface:

```
   Interface
   |     |
   v     v
ApplicationInterface
   |     |
   v     v
DirectApplicInterface
   |     |
   v     v
TestDriverInterface
```

Public Member Functions

- TestDriverInterface (const ProblemDescDB &problem_db)
  constructor
- ~TestDriverInterface ()
  destructor

Protected Member Functions

- virtual int derived_map_ac (const Dakota::String &ac_name)
  execute an analysis code portion of a direct evaluation invocation
Private Member Functions

- int cantilever ()
  scaled cantilever test function for optimization
- int mod_cantilever ()
  unscaled cantilever test function for UQ
- int cyl_head ()
  the cylinder head constrained optimization test fn
- int multimodal ()
  multimodal UQ test function
- int log_ratio ()
  the log_ratio UQ test function
- int short_column ()
  the short_column UQ/OUU test function
- int lf_short_column ()
  a low fidelity short_column test function
- int mf_short_column ()
  alternate short_column formulations for multifidelity or model form studies
- int alternate_short_column_forms (int form)
  helper fn for alternate forms
- int side_impact_cost ()
  the side_impact_cost UQ/OUU test function
- int side_impact_perf ()
  the side_impact_perf UQ/OUU test function
- int rosenbrock ()
  the Rosenbrock optimization and least squares test fn
- int modified_rosenbrock ()
  the modified Rosenbrock optimization and least squares test fn. The modification is the addition of an \( \sin^2 x \) term so that function can not be exactly approximated by a low degree polynomial
- int generalized_rosenbrock ()
  \(n\)-dimensional Rosenbrock (Schittkowski)
- int extended_rosenbrock ()
  \(n\)-dimensional Rosenbrock (Nocedal/Wright)
- int lf_rosenbrock ()
  a low fidelity version of the Rosenbrock function
- int extra_lf_rosenbrock ()
  an extra low fidelity version of the Rosenbrock function
- int mfs_rosenbrock ()
  alternate Rosenbrock formulations for multifidelity or model form studies
- int lf_poly_prod ()
  modified low fidelity Rosenbrock to test SBO with hierarchical approximations
- int poly_prod ()
  modified low fidelity Rosenbrock to test SBO with hierarchical approximations
- `int gerstner ()`
  
  the isotropic/anisotropic Gerstner test function family

- `int scalable_gerstner ()`
  
  scalable versions of the Gerstner test family

- `void get_genz_coefficients (int num_dims, Real factor, int c_type, RealVector &c, RealVector &w)`
  
  define coefficients needs for genz model

- `int genz ()`
  
  scalable test functions from the Genz test suite

- `int damped_oscillator ()`
  
  1d-6d that returns field values (ode solution)

- `int steady_state_diffusion_1d ()`
  
  solve the 1d steady-state diffusion eqn < with uncertain field diffusivity

- `int transient_diffusion_1d ()`
  
  solve the 1d transient diffusion equation < with uncertain scalar diffusivity

- `int predator_prey ()`

- `int steel_column_cost ()`
  
  solve a predator prey population dynamics model

- `int steel_column_perf ()`
  
  the steel_column_perf UQ/OUU test function

- `int sobol_rational ()`
  
  Sobol SA rational test function.

- `int sobol_g_function ()`
  
  Sobol SA discontinuous test function.

- `int sobol_ishigami ()`
  
  Sobol SA transcendental test function.

- `int text_book ()`
  
  the text_book constrained optimization test function

- `int text_book1 ()`
  
  portion of text_book() evaluating the objective fn

- `int text_book2 ()`
  
  portion of text_book() evaluating constraint 1

- `int text_book3 ()`
  
  portion of text_book() evaluating constraint 2

- `int text_book_ouu ()`
  
  the text_book_ouu OUU test function

- `int scalable_text_book ()`
  
  scalable version of the text_book test function

- `int scalable_monomials ()`
  
  simple monomials for UQ exactness testing

- `int mogatest1 ()`
  
  MOP2 from Van Veldhuizen, pp. 5-13.

- `int mogatest2 ()`
  
• int mogastest3 ()
  Srinivas' from Van Veldhuizen, pp. B-5.
• int illumination ()
  illumination example in Boyd as a general < minimization problem
• int barnes ()
  barnes test for SBO performance from Rodriguez, < Perez, Renaud, et al.
• int barnes lf ()
  lo-fi barnes test for SBO performance
• void herbie1D (size_t der_mode, Real xc_loc, std::vector<Real> &w and ders)
  1D components of herbie function
• void smooth_herbie1D (size_t der_mode, Real xc_loc, std::vector<Real> &w and ders)
  1D components of smooth herbie function
• void shubert1D (size_t der_mode, Real xc_loc, std::vector<Real> &w and ders)
  1D components of shubert function
• int herbie ()
  returns the N-D herbie function
• int smooth_herbie ()
  returns the N-D smooth herbie function
• int shubert ()
  returns the N-D shubert function
• int bayes_linear ()
  Scalable test function for Bayesian methods, to estimate parameters.
• void separable_combine (Real mult_scale_factor, std::vector<Real> &w, std::vector<Real> &d1w, std::vector<Real> &d2w)
  utility to combine components of separable fns
• Real levenshtein_distance (const String &v)
  Compute Levenshtein distance between v and LEV_REF.
• int salinas ()
  direct interface to the SALINAS structural dynamics code
• int mc_api_run ()
  direct interface to ModelCenter via API, HKIM 4/3/03
• int aniso_quad_form ()
  1-D function using a anisotropic quadratic < form

Static Private Attributes
• static StringRealMap levenshteinDistanceCache
  Cache results of Levenshtein distance calc for efficiency.

Additional Inherited Members

13.204.1 Detailed Description
Specialization of DirectApplicInterface to embed algebraic test function drivers directly in Dakota
13.204.2 Member Function Documentation

```cpp
int derived_map_ac ( const Dakota::String & ac_name ) [protected], [virtual]
```

execute an analysis code portion of a direct evaluation invocation

Derived map to evaluate a particular built-in test analysis function

Reimplemented from DirectApplicInterface.

References Dakota::abort_handler(), ApplicationInterface::analysisServerId, TestDriverInterface::aniso_quad_form(), TestDriverInterface::barnes(), TestDriverInterface::barnes_if(), TestDriverInterface::bayes_linear(), TestDriverInterface::cantilever(), TestDriverInterface::cyl_head(), TestDriverInterface::damped_oscillator(), DirectApplicInterface::driverTypeMap, TestDriverInterface::extended_rosenbrock(), TestDriverInterface::extra_if_rosenbrock(), TestDriverInterface::generalized_rosenbrock(), TestDriverInterface::genz(), TestDriverInterface::gerstner(), TestDriverInterface::herbie(), TestDriverInterface::illumination(), TestDriverInterface::lf_poly_prod(), TestDriverInterface::lf_rosenbrock(), TestDriverInterface::lf_short_column(), TestDriverInterface::log_ratio(), TestDriverInterface::mc_api_run(), TestDriverInterface::mf_rosenbrock(), TestDriverInterface::mf_short_column(), TestDriverInterface::modified_rosenbrock(), TestDriverInterface::mogatest1(), TestDriverInterface::mogatest2(), TestDriverInterface::mogatest3(), TestDriverInterface::multimodal(), TestDriverInterface::poly_prod(), TestDriverInterface::rosenbrock(), TestDriverInterface::scalable_gerstner(), TestDriverInterface::scalable_monomials(), TestDriverInterface::scalable_text_book(), TestDriverInterface::short_column(), TestDriverInterface::shubert(), TestDriverInterface::side_impact_cost(), TestDriverInterface::side_impact_perf(), TestDriverInterface::smooth_herbie(), TestDriverInterface::sobol_g_function(), TestDriverInterface::sobol_ishigami(), TestDriverInterface::sobol_rational(), TestDriverInterface::steady_state_diffusion_1d(), TestDriverInterface::steel_column_cost(), TestDriverInterface::steel_column_perf(), TestDriverInterface::text_book1(), TestDriverInterface::text_book2(), TestDriverInterface::text_book3(), TestDriverInterface::text_book_out(), and TestDriverInterface::transient_diffusion_1d().

```cpp
int lf_poly_prod ( ) [private]
```

modified low fidelity Rosenbrock to test SBO with < hierarchical approximations

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface::hessFlag, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

```cpp
int poly_prod ( ) [private]
```

modified low fidelity Rosenbrock to test SBO with < hierarchical approximations

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface::hessFlag, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

```cpp
int steady_state_diffusion_1d ( ) [private]
```

solve the 1d steady-state diffusion eqn < with uncertain field diffusivity

Solve the 1D diffusion equation with an uncertain variable coefficient using the spectral Chebyshev collocation method.
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\[ \text{del}(k \text{ del}(u)) = f \text{ on } [0,1] \text{ subject to } u(0) = 0 \ u(1) = 0 \]

Here we set \( f = -1 \) and \( k = 1 + 4. + \sum_{d=1}^{\text{num}\_\text{dims}} \left| \frac{\cos(2\pi d x)}{\pi d} \right|^2 z[d] \) where \( z[d] \) are random variables, typically i.i.d uniform[-1,1].

References Dakota::NPOS, Dakota::abort_handler(), Dakota::find_index(), DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface::hessFlag, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numADIV, DirectApplicInterface::numFns, DirectApplicInterface::numVars, DirectApplicInterface::xC, DirectApplicInterface::xDI, DirectApplicInterface::xDILabels, DirectApplicInterface::xDR, DirectApplicInterface::xDS, and DirectApplicInterface::xDSLabs.

Referenced by TestDriverInterface::derived_map_ac().

int steel_column_cost( ) [private]

solve a predator prey population dynamics model

the steel_column_cost UQ/OUU test function

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, DirectApplicInterface::numVars, DirectApplicInterface::varTypeDVV, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

int barnes( ) [private]

barnes test for SBO performance from Rodriguez, Perez, Renaud, et al.

barnes test for SBO performance from Rodriguez, Perez, Renaud, et al.

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

int barnes_lf( ) [private]

lo-fi barnes test for SBO performance

lo-fi barnes test for SBO performance from Rodriguez, Perez, Renaud, et al.

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

void herbie1D( size_t der_mode, Real xc_loc, std::vector< Real >& w_and_ders ) [private]

1D components of herbie function

1D Herbie function and its derivatives (apart from a multiplicative factor)

Referenced by TestDriverInterface::herbie().
void smooth_herbie1D ( size_t der_mode, Real xc_loc, std::vector< Real > & w_and_ders ) [private]

1D components of smooth_herbie function
1D Smoothed Herbie = 1D Herbie minus the high frequency sine term, and its derivatives (apart from a multiplicative factor)
Referenced by TestDriverInterface::smooth_herbie().

void shubert1D ( size_t der_mode, Real xc_loc, std::vector< Real > & w_and_ders ) [private]

1D components of shubert function
1D Shubert function and its derivatives (apart from a multiplicative factor)
Referenced by TestDriverInterface::shubert().

int herbie ( ) [private]
returns the N-D herbie function
N-D Herbie function and its derivatives.
References DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, TestDriverInterface::herbie1D(), DirectApplicInterface::numDerivVars, DirectApplicInterface::numVars, TestDriverInterface::separable_combine(), and DirectApplicInterface::xC.
Referenced by TestDriverInterface::derived_map_ac().

int smooth_herbie ( ) [private]
returns the N-D smooth herbie function
N-D Smoothed Herbie function and its derivatives.
References DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::numDerivVars, DirectApplicInterface::numVars, TestDriverInterface::separable_combine(), and DirectApplicInterface::xC.
Referenced by TestDriverInterface::derived_map_ac().

void separable_combine ( Real mult_scale_factor, std::vector< Real > & w, std::vector< Real > & d1w, std::vector< Real > & d2w ) [private]

utility to combine components of separable functions
this function combines N 1D functions and their derivatives to compute a N-D separable function and its derivatives, logic is general enough to support different 1D functions in different dimensions (can mix and match)
References DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::numDerivVars, and DirectApplicInterface::xC.
Referenced by TestDriverInterface::herbie(), TestDriverInterface::shubert(), and TestDriverInterface::smooth_herbie().

Real levenshtein_distance ( const String & v ) [private]

Compute Levenshtein distance between v and LEV_REF.
Levenshtein distance is the number of changes (single character
References Dakota::LEV_REF, and TestDriverInterface::levenshteinDistanceCache.
Referenced by TestDriverInterface::text_book1(), TestDriverInterface::text_book2(), and TestDriverInterface::text_book3().
int mc_api_run ( ) [private]
direct interface to ModelCenter via API, HKIM 4/3/03
The ModelCenter interface doesn’t have any specific construct vs. run time functions. For now, we manage it along with the integrated test drivers
References Dakota: abort_handler(), DirectApplicInterface::analysisComponents, DirectApplicInterface::analysisDriverIndex, Dakota::dc_print, DirectApplicInterface::directFnASV, Interface::fnLabels, DirectApplicInterface::fnVals, Dakota::mc_ptr_int, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADR, DirectApplicInterface::numFns, DirectApplicInterface::xC, DirectApplicInterface::xCLabels, DirectApplicInterface::xDI, DirectApplicInterface::xDILabels, DirectApplicInterface::xDR, and DirectApplicInterface::xDRLabels.
Referenced by TestDriverInterface::derived_map_ac().
The documentation for this class was generated from the following files:
• TestDriverInterface.hpp
• TestDriverInterface.cpp

13.205 TrackerHTTP Class Reference
TrackerHTTP: a usage tracking module that uses HTTP/HTTPS via the curl library.

Classes
• struct Server
  struct to hold tracker/proxy pairs

Public Member Functions
• TrackerHTTP ( )
  default constructor is allowed, but doesn’t generate output
• TrackerHTTP (int world_rank=0)
  standard constructor with ProblemDescDB, rank
• ~TrackerHTTP ( )
  destructor to free handles
• void post_start (ProblemDescDB &problem_db)
  post the start of an analysis and archive start time
• void post_finish (unsigned runtime=0)
  post the completion of an analysis including elapsed time

Private Member Functions
• void initialize (int world_rank=0)
  shared initialization functions across constructors
• void url_add_field (std::string &url, const char *keyword, const std::string &value, bool delimit=true) const
  append keyword/value pair to url in GET style (with &keyword=value); set delimit = false to omit the &
• void build_default_data (std::string &url, std::time_t &rawtime, const std::string &mode) const
construct URL with shared information for start/finish

• void send_data_using_get (const std::string &urltopost) const
transmit data to the web server using GET

• void send_data_using_post (const std::string &datatopost)
  POST separate location and query; datatopost = "name=daniel&project=curl".

• void split_string (const std::string &s, const char &delim, std::vector<std::string> &elems)
  Split a string on a delimiter and place tokens in elems.

• void parse_tracking_string (const std::string &dt)
  Populate serverList with tracker and proxy URLs from dt.

• void populate_method_list (ProblemDescDB &problem_db)
  extract list of methods from problem database

• std::string get_uid () const
  get the real user ID

• std::string get_username () const
  get the username as reported by the environment

• std::string get_hostname () const
  get the system hostname

• std::string get_os () const
  get the operating system

• std::string get_datetime (const std::time_t &rawtime) const
  get the date and time as a string YYYYMMDDHHMMSS

Private Attributes

• CURL * curlPtr
  pointer to the curl handler instance

• FILE * devNull
  pointer to /dev/null

• std::list<Server> serverList
  List of servers to try (tracker and proxy)

• long timeoutSeconds
  seconds until the request will timeout (may have issues with signals)

• std::string methodList
  list of active methods

• std::string dakotaVersion
  DAKOTA version.

• std::time_t startTime
  cached starting time in raw seconds

• short outputLevel
  verbosity control

13.205.1 Detailed Description

TrackerHTTP: a usage tracking module that uses HTTP/HTTPS via the curl library.
13.205.2 Member Function Documentation

void send_data_using_get ( const std::string & urltopost ) const [private]
transmit data to the web server using GET
whole url including location&fields
References TrackerHTTP::curlPtr, and TrackerHTTP::outputLevel.

void send_data_using_post ( const std::string & datatopost ) [private]
POST separate location and query; datatopost="name=daniel&project=curl".
separate location and query; datatopost="name=daniel&project=curl"
References TrackerHTTP::curlPtr, TrackerHTTP::outputLevel, and TrackerHTTP::serverList.
Referenced by TrackerHTTP::post_finish(), and TrackerHTTP::post_start().
The documentation for this class was generated from the following files:
- TrackerHTTP.hpp
- TrackerHTTP.cpp

13.206 UsageTracker Class Reference

Lightweight class to manage conditionally active Curl-based HTTP tracker via PIMPL.

Public Member Functions
- UsageTracker ()
  default construction: no output
- UsageTracker (int world_rank)
  standard constructor: will output on rank 0
- void post_start (ProblemDescDB &problem_db)
  post the start of an analysis and archive start time
- void post_finish (unsigned runtime=0)
  post the completion of an analysis including elapsed time

Private Member Functions
- UsageTracker (const UsageTracker &)
  copy construction is disallowed

Private Attributes
- boost::shared_ptr< TrackerHTTP > pTrackerHTTP
  posts usage data to Web server; using shared_ptr due to potentially incomplete type and requirements for checked-
  _delete in debug builds (scoped_ptr would suffice)

13.206.1 Detailed Description

Lightweight class to manage conditionally active Curl-based HTTP tracker via PIMPL.
All conditional compilation in managed in the cpp file; all operations are no-op in this wrapper if not enabling tracking...
13.206.2 Constructor & Destructor Documentation

UsageTracker ( int world_rank )

standard constructor; will output on rank 0

standard constructor; will output on rank 0 and only initializes if tracking compiled in and not disable by environment

References UsageTracker::pTrackerHTTP.

The documentation for this class was generated from the following files:

- UsageTracker.hpp
- UsageTracker.cpp

13.207 Var_icheck Struct Reference

structure for verifying bounds and initial point for string-valued vars

Public Attributes

- const char * name
- size_t DataVariablesRep::* n
- void(* vgen)(DataVariablesRep *, size_t)
- IntVector DataVariablesRep::* L
- IntVector DataVariablesRep::* U
- IntVector DataVariablesRep::* V
- StringArray DataVariablesRep::* Lbl

13.207.1 Detailed Description

structure for verifying bounds and initial point for string-valued vars

structure for verifying bounds and initial point for integer-valued vars

The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

13.208 Var_rcheck Struct Reference

structure for verifying bounds and initial point for real-valued vars

Public Attributes

- const char * name
- size_t DataVariablesRep::* n
- void(* vgen)(DataVariablesRep *, size_t)
- RealVector DataVariablesRep::* L
- RealVector DataVariablesRep::* U
- RealVector DataVariablesRep::* V
- StringArray DataVariablesRep::* Lbl
13.208.1 Detailed Description

structure for verifying bounds and initial point for real-valued vars

The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

13.209 Variables Class Reference

Base class for the variables class hierarchy.

Inheritance diagram for Variables:

```
Variables
   ▼
  |  
 MixedVariables RelaxedVariables
```

Public Member Functions

- **Variables ()**
  
  default constructor

- **Variables (const ProblemDescDB &problem_db)**
  
  standard constructor (explicit disallows its use for implicit type conversion)

- **Variables (const SharedVariablesData &svd)**
  
  alternate constructor for instantiations on the fly (explicit disallows its use for implicit type conversion)

- **Variables (const Variables &vars)**
  
  copy constructor

- **virtual ~Variables ()**
  
  destructor

- **Variables operator= (const Variables &vars)**
  
  assignment operator

- **virtual void read (std::istream &s)**
  
  read a variables object from an std::istream

- **virtual void write (std::ostream &s, unsigned short vars_part=ALL_VARS) const**
  
  write a variables object to an std::ostream, e.g., the console, optionally specifying which partition (all/active/inactive)

- **virtual void write_aprepro (std::ostream &s) const**
  
  write a variables object to an std::ostream in aprepro format, e.g., a parameters file

- **virtual void read.annotated (std::istream &s)**
  
  read a variables object in annotated format from an istream

- **virtual void write.annotated (std::ostream &s) const**
  
  write a variables object in annotated format to an std::ostream

- **virtual void read.tabular (std::istream &s, unsigned short vars_part=ALL_VARS)**
  
  read a variables object in tabular format from an istream, optionally specifying which partition (all/active/inactive)

- **virtual void write.tabular (std::ostream &s, unsigned short vars_part=ALL_VARS) const**
write a variables object in tabular format to an std::ostream, optionally specifying which partition (all/active/inactive)

- virtual void write_tabular_labels (std::ostream &s, unsigned short vars_part=ALL_VARS) const

write the labels in input spec order to a std::ostream, optionally specifying which partition (all/active/inactive)

- virtual void read (MPIUnpackBuffer &s)

read a variables object from a packed MPI buffer

- virtual void write (MPIPackBuffer &s) const

write a variables object to a packed MPI buffer

- size_t tv () const
  total number of vars

- size_t cv () const
  number of active continuous vars

- size_t cv_start () const
  start index of active continuous vars

- size_t div () const
  number of active discrete int vars

- size_t div_start () const
  start index of active discrete int vars

- size_t dsv () const
  number of active discrete string vars

- size_t dsv_start () const
  start index of active discrete string vars

- size_t drv () const
  number of active discrete real vars

- size_t drv_start () const
  start index of active discrete real vars

- size_t icv () const
  number of inactive continuous vars

- size_t icv_start () const
  start index of inactive continuous vars

- size_t idiv () const
  number of inactive discrete int vars

- size_t idiv_start () const
  start index of inactive discrete int vars

- size_t idsv () const
  number of inactive discrete string vars

- size_t idsv_start () const
  start index of inactive discrete string vars

- size_t idrv () const
  number of inactive discrete real vars

- size_t idrv_start () const
  start index of inactive discrete real vars

- size_t acv () const
  total number of continuous vars
- `size_t adiv () const`  
  total number of discrete integer vars
- `size_t adsv () const`  
  total number of discrete string vars
- `size_t adrv () const`  
  total number of discrete real vars
- `const SharedVariablesData & shared_data () const`  
  return sharedVarsData
- `SharedVariablesData & shared_data ()`  
  return sharedVarsData
- `void shape ()`  
  shape a Variables object based on sharedVarsData
- `void reshape ()`  
  reshape an existing Variables object based on updated sharedVarsData
- `Real continuous_variable (size_t index) const`  
  return an active continuous variable
- `const RealVector & continuous_variables () const`  
  return the active continuous variables (Note: returns a view by const reference, but initializing a RealVector from this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable view, use continuous_variables_view())
- `void continuous_variable (Real c_var, size_t index)`  
  set an active continuous variable
- `void continuous_variables (const RealVector &c_vars)`  
  set the active continuous variables
- `int discrete_int_variable (size_t index) const`  
  return an active discrete integer variable
- `const IntVector & discrete_int_variables () const`  
  return the active discrete integer variables (Note: returns a view by const reference, but initializing an IntVector from this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable view, use discrete_int_variables_view())
- `void discrete_int_variable (int di_var, size_t index)`  
  set an active discrete integer variable
- `void discrete_int_variables (const IntVector &di_vars)`  
  set the active discrete integer variables
- `const String & discrete_string_variable (size_t index) const`  
  return an active discrete string variable
- `StringMultiArrayConstView discrete_string_variables () const`  
  return the active discrete string variables (Note: returns a view by const reference, but initializing a StringArray from this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable view, use discrete_string_variables_view())
- `void discrete_string_variable (const String &ds_var, size_t index)`  
  set an active discrete string variable
- `void discrete_string_variables (StringMultiArrayConstView ds_vars)`  
  set the active discrete string variables
• Real \texttt{discrete\_real\_variable} (size\_t index) const
  return an active discrete real variable
• const RealVector \& \texttt{discrete\_real\_variables} () const
  return the active discrete real variables (Note: returns a view by const reference, but initializing a RealVector from
  this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable
  view, use \texttt{discrete\_real\_variables}\_view())
• void \texttt{discrete\_real\_variable} (Real dr\_var, size\_t index)
  set an active discrete real variable
• void \texttt{discrete\_real\_variables} (const RealVector \&dr\_vars)
  set the active discrete real variables
• void \texttt{active\_variables} (const Variables \&vars)
  copy the active cv/div/dsv/drv variables from vars
• void \texttt{all\_variables} (const Variables \&vars)
  copy all cv/div/dsv/drv variables from vars
• RealVector \& \texttt{continuous\_variables}\_view ()
  return a mutable view of the active continuous variables
• IntVector \& \texttt{discrete\_int\_variables}\_view ()
  return a mutable view of the active discrete integer variables
• StringMultiArrayView \texttt{discrete\_string\_variables}\_view ()
  return a mutable view of the active discrete string variables
• RealVector \& \texttt{discrete\_real\_variables}\_view ()
  return a mutable view of the active discrete real variables
• StringMultiArrayConstView \texttt{continuous\_variable\_labels} () const
  return the active continuous variable labels
• void \texttt{continuous\_variable\_labels} (StringMultiArrayConstView cv\_labels)
  set the active continuous variable labels
• void \texttt{continuous\_variable\_label} (const String \&cv\_label, size\_t index)
  set an active continuous variable label
• StringMultiArrayConstView \texttt{discrete\_int\_variable\_labels} () const
  return the active discrete integer variable labels
• void \texttt{discrete\_int\_variable\_labels} (StringMultiArrayConstView div\_labels)
  set the active discrete integer variable labels
• void \texttt{discrete\_int\_variable\_label} (const String \&div\_label, size\_t index)
  set an active discrete integer variable label
• StringMultiArrayConstView \texttt{discrete\_string\_variable\_labels} () const
  return the active discrete string variable labels
• void \texttt{discrete\_string\_variable\_labels} (StringMultiArrayConstView dsv\_labels)
  set the active discrete string variable labels
• void \texttt{discrete\_string\_variable\_label} (const String \&dsv\_label, size\_t index)
  set an active discrete string variable label
• StringMultiArrayConstView \texttt{discrete\_real\_variable\_labels} () const
  return the active discrete real variable labels
• void \texttt{discrete\_real\_variable\_labels} (StringMultiArrayConstView drv\_labels)
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set the active discrete real variable labels
• void discrete_real_variable_label (const String &drv_label, size_t index)
  set an active discrete real variable label

UShortMultiArrayConstView continuous_variable_types () const
  return the active continuous variable types
• void continuous_variable_types (UShortMultiArrayConstView cv_types)
  set the active continuous variable types

UShortMultiArrayConstView discrete_int_variable_types () const
  return the active discrete integer variable types
• void discrete_int_variable_types (UShortMultiArrayConstView div_types)
  set the active discrete integer variable types

UShortMultiArrayConstView discrete_string_variable_types () const
  return the active discrete string variable types
• void discrete_string_variable_types (UShortMultiArrayConstView dsv_types)
  set the active discrete string variable types

UShortMultiArrayConstView discrete_real_variable_types () const
  return the active discrete real variable types
• void discrete_real_variable_types (UShortMultiArrayConstView drv_types)
  set the active discrete real variable types

SizetMultiArrayConstView continuous_variable_ids () const
  return the active continuous variable position identifiers
• void continuous_variable_ids (SizetMultiArrayConstView cv_ids)
  set the active continuous variable position identifiers

const RealVector & inactive_continuous_variables () const
  return the inactive continuous variables
• void inactive_continuous_variables (const RealVector &ic_vars)
  set the inactive continuous variables

const IntVector & inactive_discrete_int_variables () const
  return the inactive discrete int variables
• void inactive_discrete_int_variables (const IntVector &idi_vars)
  set the inactive discrete int variables
• void inactive_discrete_int_variable (int idi_var, size_t index)
  set an inactive discrete int variable
• StringMultiArrayConstView inactive_discrete_string_variables () const
  return the inactive discrete string variables
• void inactive_discrete_string_variables (StringMultiArrayConstView ids_vars)
  set the inactive discrete string variables
• void inactive_discrete_string_variable (const String &ids_var, size_t index)
  set an inactive discrete string variable
• const RealVector & inactive_discrete_real_variables () const
  return the inactive discrete real variables
• void inactive_discrete_real_variables (const RealVector &idr_vars)
  set the inactive discrete real variables
• void inactive_discrete_real_variable (Real idr_var, size_t index)
  set an inactive discrete real variable
• StringMultiArrayConstView inactive_continuous_variable_labels () const
  return the inactive continuous variable labels
• void inactive_continuous_variable_labels (StringMultiArrayConstView ic_vars)
  set the inactive continuous variable labels
• StringMultiArrayConstView inactive_discrete_int_variable_labels () const
  return the inactive discrete variable labels
• void inactive_discrete_int_variable_labels (StringMultiArrayConstView idi_vars)
  set the inactive discrete variable labels
• StringMultiArrayConstView inactive_discrete_string_variable_labels () const
  return the inactive discrete string variable labels
• void inactive_discrete_string_variable_labels (StringMultiArrayConstView ids_vars)
  set the inactive discrete string variable labels
• StringMultiArrayConstView inactive_discrete_real_variable_labels () const
  return the inactive discrete real variable labels
• void inactive_discrete_real_variable_labels (StringMultiArrayConstView idr_vars)
  set the inactive discrete real variable labels
• UShortMultiArrayConstView inactive_continuous_variable_types () const
  return the inactive continuous variable types
• UShortMultiArrayConstView inactive_discrete_int_variable_types () const
  return the inactive discrete integer variable types
• UShortMultiArrayConstView inactive_discrete_string_variable_types () const
  return the inactive discrete string variable types
• UShortMultiArrayConstView inactive_discrete_real_variable_types () const
  return the inactive discrete real variable types
• SizetMultiArrayConstView inactive_continuous_variable_ids () const
  return the inactive continuous variable position identifiers
• const RealVector & all_continuous_variables () const
  returns a single array with all continuous variables
• void all_continuous_variables (const RealVector &ac_vars)
sets all continuous variables using a single array

• void all_continuous_variable (Real ac_var, size_t index)
  set a variable within the all continuous array

• const IntVector & all_discrete_int_variables () const
  returns a single array with all discrete variables

• void all_discrete_int_variables (const IntVector &adi_vars)
  sets all discrete variables using a single array

• void all_discrete_int_variable (int adi_var, size_t index)
  set a variable within the all discrete array

• StringMultiArrayConstView all_discrete_string_variables () const
  returns a single array with all discrete variables

• void all_discrete_string_variables (StringMultiArrayConstView ads_vars)
  sets all discrete variables using a single array

• void all_discrete_string_variable (const String &ads_var, size_t index)
  set a variable within the all discrete array

• const RealVector & all_discrete_real_variables () const
  returns a single array with all discrete variables

• void all_discrete_real_variables (const RealVector &adr_vars)
  sets all discrete variables using a single array

• void all_discrete_real_variable (Real adr_var, size_t index)
  set a variable within the all discrete array

• void as_vector (const StringSetArray &dss_vals, RealVector &var_values)
  get the active variables as a vector of reals, converting string values to zero-based set indices

• StringMultiArrayView all_continuous_variable_labels () const
  returns a single array with all continuous variable labels

• void all_continuous_variable_labels (StringMultiArrayConstView acv_labels)
  sets all continuous variable labels using a single array

• void all_continuous_variable_label (const String &acv_label, size_t index)
  set a label within the all continuous label array

• StringMultiArrayView all_discrete_int_variable_labels () const
  returns a single array with all discrete variable labels

• void all_discrete_int_variable_labels (StringMultiArrayConstView adiv_labels)
  sets all discrete variable labels using a single array

• void all_discrete_int_variable_label (const String &adiv_label, size_t index)
  set a label within the all discrete label array

• StringMultiArrayView all_discrete_string_variable_labels () const
  returns a single array with all discrete variable labels

• void all_discrete_string_variable_labels (StringMultiArrayConstView adsv_labels)
  sets all discrete variable labels using a single array

• void all_discrete_string_variable_label (const String &adsv_label, size_t index)
  set a label within the all discrete label array

• StringMultiArrayView all_discrete_real_variable_labels () const
  returns a single array with all discrete variable labels
• void **all_discrete_real_variable_labels** (StringMultiArrayConstView adrv_labels)
  sets all discrete variable labels using a single array
• void **all_discrete_real_variable_label** (const String &adrv_label, size_t index)
  set a label within the all discrete label array
• UShortMultiArrayConstView **all_continuous_variable_types** () const
  return all continuous variable types
• UShortMultiArrayConstView **all_discrete_int_variable_types** () const
  return all discrete variable types
• UShortMultiArrayConstView **all_discrete_string_variable_types** () const
  return all discrete variable types
• UShortMultiArrayConstView **all_discrete_real_variable_types** () const
  return all discrete variable types
• SizeMultiArrayConstView **all_continuous_variable_ids** () const
  return all continuous variable position identifiers
• Variables **copy** (bool deep_svd=false) const
  a deep variables copy for use in history mechanisms (SharedVariablesData uses a shallow copy by default)
• const std::pair< short, short > & **view** () const
  returns variablesView
• std::pair< short, short > **get_view** (const ProblemDescDB &problem_db) const
  defines variablesView from problem_db attributes
• void **inactive_view** (short view2)
  sets the inactive view based on higher level (nested) context
• const String & **variables_id** () const
  returns the variables identifier string
• const SizeMultiArray & **variables_components_totals** () const
  returns the number of variables for each of the constitutive components
• bool **is_null** () const
  function to check variablesRep (does this envelope contain a letter)

**Protected Member Functions**

• **Variables** (BaseConstructor, const ProblemDescDB &problem_db, const std::pair< short, short > &view)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
• **Variables** (BaseConstructor, const SharedVariablesData &svd)
  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
• void **build_views** ()
  construct active/inactive views of all variables arrays
• void **build_active_views** ()
  construct active views of all variables arrays
• void **build_inactive_views** ()
  construct inactive views of all variables arrays
Protected Attributes

- **SharedVariablesData sharedVarsData**
  - reference-counted instance of shared variables data: id's, labels, counts
- **RealVector allContinuousVars**
  - array combining all of the continuous variables
- **IntVector allDiscreteIntVars**
  - array combining all of the discrete integer variables
- **StringMultiArray allDiscreteStringVars**
  - array combining all of the discrete string variables
- **RealVector allDiscreteRealVars**
  - array combining all of the discrete real variables
- **RealVector continuousVars**
  - the active continuous variables array view
- **IntVector discreteIntVars**
  - the active discrete integer variables array view
- **RealVector discreteRealVars**
  - the active discrete real variables array view
- **RealVector inactiveContinuousVars**
  - the inactive continuous variables array view
- **IntVector inactiveDiscreteIntVars**
  - the inactive discrete integer variables array view
- **RealVector inactiveDiscreteRealVars**
  - the inactive discrete real variables array view

Private Member Functions

- **Variables * get_variables (const ProblemDescDB &problem_db)**
  - Used by the standard envelope constructor to instantiate the correct letter class.
- **Variables * get_variables (const SharedVariablesData &svd) const**
  - Used by the alternate envelope constructors, by read functions, and by copy() to instantiate a new letter class.
- **short method_map (short view_spec, bool relaxed) const**
  - infer domain from method selection
- **short method_domain (const ProblemDescDB &problem_db) const**
  - infer domain from method selection
- **short method_view (const ProblemDescDB &problem_db) const**
  - infer view from method selection
- **short response_view (const ProblemDescDB &problem_db) const**
  - infer view from type of response data set
- **void check_view_compatibility ()**
  - perform sanity checks on view.first and view.second after update
- **template<class Archive>**
  - **void load (Archive &, const unsigned int version)**
    - read a Variables object from an archive
13.209. VARIABLES CLASS REFERENCE

- template<class Archive >
  void save (Archive &ar, const unsigned int version) const
  write a Variables object to an archive

- BOOST_SERIALIZATION_SPLIT_MEMBER () Variables *variablesRep
  pointer to the letter (initialized only for the envelope)

Private Attributes

- int referenceCount
  number of objects sharing variablesRep

Friends

- class boost::serialization::access
  for serializing private data members
- bool operator==(const Variables &vars1, const Variables &vars2)
  strict equality operator (for boost hash-based lookups)
- bool operator!=(const Variables &vars1, const Variables &vars2)
  strict inequality operator
- bool nearby(const Variables &vars1, const Variables &vars2, Real rel_tol)
  tolerance-based equality operator
- std::size_t hash_value (const Variables &vars)
  hash_value

13.209.1 Detailed Description

Base class for the variables class hierarchy.

The Variables class is the base class for the class hierarchy providing design, uncertain, and state variables for continuous and discrete domains within a Model. Using the fundamental arrays from the input specification, different derived classes define different views of the data. For memory efficiency and enhanced polymorphism, the variables hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Variables) serves as the envelope and one of the derived classes (selected in Variables::get_variables()) serves as the letter.

13.209.2 Member Function Documentation

StringMultiArrayView discrete_string_variables_view () [inline]
return a mutable view of the active discrete string variables
same as discrete_string_variables(), except mutable view
References Variables::allDiscreteStringVars, SharedVariablesData::dsv(), SharedVariablesData::dsv_start(), and Variables::sharedVarsData.

The documentation for this class was generated from the following file:

- DakotaVariables.hpp
13.210 Verification Class Reference

Base class for managing common aspects of verification studies.

Inheritance diagram for Verification:

```
Verification
   |                        | Analyzer
   |                        |   |
   |                        |   |
   |                        |   |
   |   Iterator             |   |
   |                        |   |
   |                        |   |
   |                        |   |
   |                        |   |
   |                        |   |
   |                        |   |
   |   RichExtrapVerification |
```

Public Member Functions
- bool resize ()
  reinitializes iterator based on new variable size

Protected Member Functions
- Verification (ProblemDescDB &problem_db, Model &model)
  constructor
- Verification (unsigned short method_name, Model &model)
  alternate constructor for instantiations "on the fly"
- ~Verification ()
  destructor
- void print_results (std::ostream &s)
  print the final iterator results

Additional Inherited Members

13.210.1 Detailed Description

Base class for managing common aspects of verification studies.

The Verification base class manages common data and functions, such as those involving ...

13.210.2 Member Function Documentation

void print_results ( std::ostream & s ) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().
Reimplemented from Analyzer.
Reimplemented in RichExtrapVerification.
References Analyzer::print_results().
Referenced by RichExtrapVerification::print_results().
The documentation for this class was generated from the following files:
- DakotaVerification.hpp
- DakotaVerification.cpp

13.211 VLint Struct Reference

structure for validating integer uncertain variable labels, bounds, values

Public Attributes
- int n
- VarLabel Var_Info::* VL
- Var_uinfo * vui
- StringArray DataVariablesRep::* Labels
- IntVector DataVariablesRep::* LowerBnds
- IntVector DataVariablesRep::* UpperBnds
- IntVector DataVariablesRep::* UncVars

13.211.1 Detailed Description

structure for validating integer uncertain variable labels, bounds, values
The documentation for this struct was generated from the following file:
- NIDRProblemDescDB.cpp

13.212 VLreal Struct Reference

structure for validating real uncertain variable labels, bounds, values

Public Attributes
- int n
- VarLabel Var_Info::* VL
- Var_uinfo * vui
- StringArray DataVariablesRep::* Labels
- RealVector DataVariablesRep::* LowerBnds
- RealVector DataVariablesRep::* UpperBnds
- RealVector DataVariablesRep::* UncVars

13.212.1 Detailed Description

structure for validating real uncertain variable labels, bounds, values
The documentation for this struct was generated from the following file:
- NIDRProblemDescDB.cpp
13.213 VLstr Struct Reference

structure for validating string uncertain variable labels, bounds, values

Public Attributes

- int n
- VarLabel Var_Info::* VL
- Var_uinfo * vui
- StringArray DataVariablesRep::* Labels
- StringArray DataVariablesRep::* LowerBnds
- StringArray DataVariablesRep::* UpperBnds
- StringArray DataVariablesRep::* UncVars

13.213.1 Detailed Description

structure for validating string uncertain variable labels, bounds, values

The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

13.214 VPSApproximation Class Reference

Derived approximation class for VPS implementation.

Inheritance diagram for VPSApproximation:

```
Approximation

VPSApproximation
```

Public Member Functions

- **VPSApproximation ()**
  *default constructor*
- **VPSApproximation (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)**
  *standard constructor (to call VPS from an input deck)*
- **VPSApproximation (const SharedApproxData &shared_data)**
  *Alternate constructor (to call VPS from another method like POF-darts)*
- **~VPSApproximation ()**
  *destructor*
- bool **VPS_execute ()**
- void **VPS_create_containers ()**
- void **VPS_retrieve_neighbors (size_t ipoint, bool update_point_neighbors)**
- void **VPS_adjust_extend_neighbors_of_all_points ()**
void VPS_extend_neighbors (size_t ipoint)
void VPS_build_local_surrogate (size_t cell_index)
double VPS_evaluate_surrogate (double *x)
void VPS_destroy_global_containers ()
void retrieve_permutations (size_t &m, size_t **perm, size_t num_dim, size_t upper_bound, bool force_-
sum_constraint, size_t sum_constraint)
void build_radial_basis_function (size_t icell)
void VPS_LS_retrieve_weights (size_t cell_index)
double evaluate_basis_function (double *x, size_t icell, size_t ibasis)
int constrained_LeastSquare (size_t n, size_t m, double **H, double *w, double *f)
double vec_dot_vec (size_t n, double *vec_a, double *vec_b)
double vec_pow_vec (size_t num_dim, double *vec_a, size_t *vec_b)
bool Cholesky (int n, double **A, double **LD)
void Cholesky_solver (int n, double **LD, double *b, double *x)
void GMRES (size_t n, double **A, double *b, double *x, double eps)
void printMatrix (size_t m, size_t n, double **M)
void initiate_random_number_generator (unsigned long x)
double generate_a_random_number ()
size_t retrieve_closest_cell (double *x)
bool trim_line_using_Hyperplane (size_t num_dim, double *st, double *end, double *qH, double *nH)
double f_test (double *x)
double *grad_f_test (double *x)
double **hessian_f_test (double *x)
void generate_poisson_disk_sample (double r)
void generate_MC_sample ()
void isocontouring (std::string file_name, bool plot_test_function, bool plot_surrogate, std::vector<
double > contours)
void isocontouring_solid (std::string file_name, bool plot_test_function, bool plot_surrogate, std::vector<
double > contours)
void plot_neighbors ()

Protected Member Functions

int min_coefficients () const
return the minimum number of samples (unknowns) required to build the derived class approximation type in num-
Vars dimensions
int num_constraints () const
return the number of constraints to be enforced via an anchor point
void build ()
built the approximation from scratch
Real value (const Variables &vars)
retrieve the predicted function value for a given parameter set
const RealVector & gradient (const Variables &vars)
retrieve the function gradient at the predicted value for a given parameter set
Real prediction_variance (const Variables &vars)
retrieve the variance of the predicted value for a given parameter set
CHAPTER 13. CLASS DOCUMENTATION

Private Types

- enum **subsurrogate** { LS, GP }
- enum **subsurrogate** basis { polynomial, radial }
- enum **testfunction** {
  SmoothHerbie, Herbie, Cone, Cross,
  UnitSphere, Linear34 }

Private Member Functions

- void **VPSmodel** build ()
  Function to compute coefficients governing the VPS surrogates.
- void **VPSmodel** apply (const RealVector &new x, bool variance_flag, bool gradients_flag)
  Function returns a response value using the VPS surface.

Private Attributes

- Real **approxValue**
  value of the approximation returned by **value**()
- Real **approxVariance**
  value of the approximation returned by **prediction_variance**()
- RealMatrix **trainPoints**
  A 2-D array (num sample sites = rows, num vars = columns) used to create the Gaussian process.
- RealMatrix **trainValues**
  An array of response values; one response value per sample site.
- size_t **numObs**
  The number of observations on which the GP surface is built.
- int **surrogateOrder**
  The order of the polynomial in each Voronoi cell.
- **subsurrogate** _**vps_subsurrogate**
- **subsurrogate** basis _**vps_subsurrogate** basis
- **testfunction** _**vps_test_function*
- double **Q** [1220]
- int **index**
- double cc
- double c
- double zc
- double zx
- double zy
- size_t **qlen**
- size_t **n_dim**
- double * _**xmin**
- double * _**xmax**
- double _**diag**
- size_t **num_inserted_points**
- double **sample_points**
13.214. VPSAPPROXIMATION CLASS REFERENCE

- double * _fval
- double ** _fgrad
- double *** _fhess
- size_t ** _sample_neighbors
- size_t ** _vps_ext_neighbors
- size_t _vps_order
- size_t _num_GMRES
- size_t * _num_cell_basis_functions
- double * _sample_vsize
- double * _vps_dfar
- double *** _sample_basis
- double _max_vsize
- double _disc_min_jump
- double _disc_min_grad
- double _f_min
- double _f_max
- size_t *** _vps_t
- double ** _vps_w
- SharedApproxData sharedData
- std::vector< Approximation > gpApproximations
- Variables gpEvalVars
- bool _use_derivatives
- bool _use_gradient
- bool _use_hessian

Static Private Attributes
- static VPSApproximation * VPSinstance
  
  pointer to the active object instance used within the static evaluator

Additional Inherited Members

13.214.1 Detailed Description

Derived approximation class for VPS implementation.

The VPSApproximation class provides a set of piecewise surrogate approximations

each of which is valid within a Voronoi cell.

13.214.2 Member Function Documentation

void VPSmodel_apply ( const RealVector & new_x, bool variance_flag, bool gradients_flag ) [private]

Function returns a response value using the VPS surface.
  
  The response value is computed at the design point specified by the RealVector function argument.
  References VPSApproximation::approxValue.
  
  Referenced by VPSApproximation::gradient(), VPSApproximation::prediction_variance(), and VPSApproximation-
  ::value().
13.214.3 Member Data Documentation

VPSApproximation * VPSInstance [static], [private]

pointer to the active object instance used within the static evaluator
default constructor

The documentation for this class was generated from the following files:

- VPSApproximation.hpp
- VPSApproximation.cpp

13.215 WorkdirHelper Class Reference

Static Public Member Functions

- static void initialize ()
  initialize (at runtime) cached values for paths and environment
- static const std::string & startup_pwd ()
  Query for dakota’s startup $PWD.
- static void change_directory (const bfs::path &new_dir)
  change current directory
- static void prepend_preferred_env_path (const std::string &extra_path)
  Prepend cached preferredEnvPath with extra_path and update $PATH environment variable.
- static void set_environment (const std::string &env_name, const std::string &env_val, bool overwrite_flag=true)
  Set an environment variable.
- static bfs::path which (const std::string &driver_name)
  Returns the bfs::path for the analysis driver, supporting typical windows filename extensions, or empty if not found.
- static bfs::path rel_to_abs (const bfs::path &subdir_path)
  get a valid absolute bfs::path to a subdirectory relative to rundir
- static StringArray tokenize_driver (const String &user_an_driver)
  tokenize a white-space separated analysis driver, respecting escapes and nested quotes
- static bool resolve_driver_path (String &an_driver)
  parse off the first whitespace-separated entry in the user’s analysis_driver, and convert it to an absolute path if it begins with ./ or ../, replacing the passed string if needed. Returns true if the first token was modified.
- static void split_wildcard (const std::string &path with wc, bfs::path &search_dir, bfs::path &wild_card)
  given a string with an optional path and a wildcard, e.g., /tmp/D*.?pp, parse it into the search path /tmp (default .) and the wildcard D*.?pp. Return wild_card as path to reducewstring conversions
- static bfs::path concat_path (const bfs::path &p_in, const String &tag)
  concatenate a string onto the end of a path
- static bfs::path system_tmp_file (const std::string &prefix)
  generate a valid temporary file name <prefix>.*%%.*%%%%%%
- static bfs::path system_tmp_path ()
  get the system tmp path, e.g., /tmp or C:
- static bool create_directory (const bfs::path &dir_path, short mkdir_option)
  Create a directory, with options for remove or error.
- static void recursive_remove (const bfs::path &rm_path, short fileop_option)
Remove a path (file, directory, or symlink) without regard to its type. Only error if existed and there’s an error in the remove.

- **static void rename** (const bfs::path &old_path, const bfs::path &new_path, short fileop_option)
  Rename a file, catching any errors and optionally warning/erroring.

- **static void link** (const StringArray &source_items, const bfs::path &dest_dir, bool overwrite)
  top-level link a list of source paths (files, directories, symlinks), potentially including wildcards, from destination_dir, which must exist

- **static void copy** (const StringArray &source_items, const bfs::path &dest_dir, bool overwrite)
  copy a list of source paths (files, directories, symlinks), potentially including wildcards into destination_dir, which must exist

- **static void prepend_path** (const StringArray &source_items)
  prepend any directories (including wildcards) found in source items to the preferred environment path; this will update cached preferred path and PATH

- **static bool check_equivalent** (const StringArray &source_items, const bfs::path &dest_dir)
  check whether any of the passed source items are filesystem equivalent to the destination path, return true if any one is equivalent to dest

- **static bool find_driver** (const StringArray &source_items, const bfs::path &search_driver)
  check whether the any of the passed source items (possibly including wildcards to be expanded) matches the passed search driver

- **static bool link** (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)
  create link from dest_dir/src_path.filename() to a single path (file, dir, link) in source directory

- **static bool recursive_copy** (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)
  recursive copy of src_path into dest_dir, with optional top-level overwrite (remove/recreate) of dest_dir/src_path.filename()

- **static bool prepend_path_item** (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)
  prepend the preferred env path with source path if it’s a directory; this will update cached preferred path and manipulate PATH

- **static bool check_equivalent** (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)
  return true if the src and dest are filesystem equivalent

- **static bool find_file** (const bfs::path &src_path, const bfs::path &search_file, bool overwrite)
  return true if the src_path is a regular file and has same filename as search_file

- **static bool file_op** (const file_op_function &file_op, const StringArray &source_paths, const bfs::path &dest_dir, bool overwrite)
  recursively perform file_op (copy, path adjust, etc.) on a list of source_paths (files, directories, symlinks), which potentially include wildcards, w.r.t. destination_dir

- **static void set_preferred_path** ()
  set/reset PATH to dakPreferredEnvPath

- **static void set_preferred_path** (const boost::filesystem::path &extra_path)
  set PATH to absolute(extra_path):dakPreferredEnvPath, without changing cached preferred PATH

- **static void reset** ()
  Resets the working directory "state" to its initial state when DAKOTA was launched.
Private Member Functions

- **WorkdirHelper ()**
  - default constructor
- **WorkdirHelper (const WorkdirHelper &)**
  - copy constructor
- **~WorkdirHelper ()**
  - destructor
- **WorkdirHelper & operator= (const WorkdirHelper &)**
  - assignment operator

Static Private Member Functions

- **static bfs::path po_which (const std::string &driver_name)**
  - Returns the bfs::path for the analysis driver - POSIX-style implementation, returns empty if not found.
- **static std::string init_startup_path ()**
  - Initializes class member, startupPATH.
- **static std::string init_preferred_env_path ()**
  - Initializes class member, dakPreferredEnvPath.
- **static std::vector<std::string> tokenize_env_path (const std::string &path)**
  - Tokenizes $PATH$ environment variable into a ”list” of directories.

Static Private Attributes

- **static std::string startupPWD = "."**
  - Value of $PWD$ var upon entry to dakota main()
- **static std::string startupPATH = "."**
  - Value of $PATH$ (PATH% on windows) var upon entry to dakota main(), omitting any leading PATH= or Path=.
- **static std::string dakPreferredEnvPath = "."**
  - Dakota preferred search PATH/Path = ":startupPWD:startupPATH”, omitting any leading PATH= or Path=.

13.215.1 Detailed Description

Utility class for cross-platform management of environment and paths. Including directory and file operations. On initialization, this class does not manipulate the present working directory, nor the PATH environment variable, but stores context to manipulate them later.

13.215.2 Member Function Documentation

```cpp
void initialize ( ) [static]
```
initialize (at runtime) cached values for paths and environment

Initialize defers calls to Boost filesystem utilities until runtime (required on some operating systems.

References WorkdirHelper::dakPreferredEnvPath, WorkdirHelper::init_preferred_env_path(), WorkdirHelper::init_startup_path(), WorkdirHelper::startupPATH, and WorkdirHelper::startupPWD.

Referenced by Environment::Environment().
void prepend_preferred_env_path ( const std::string & extra_path ) [static]
Prepend cached preferredEnvPath with extra_path and update $PATH environment variable.
Overwrites $PATH with an additional directory prepended, typically for the purpose of ensuring templatedir
is in the $PATH; updates cached preferred PATH and environment PATH, so exercise caution with repeated calls.
References WorkdirHelper::dakPreferredEnvPath, WorkdirHelper::set_environment(), and WorkdirHelper::startup-
PWD.
Referenced by WorkdirHelper::prepend_path_item().

bfs::path which ( const std::string & driver_name ) [static]
Returns the bfs::path for the analysis driver, supporting typical windows filename extensions, or empty if not found.
Uses string representing $PATH to locate an analysis driver on the host computer. Returns the path to the
driver (as a string)
This version is a wrapper over the "plain ol’ which" implementation, allowing an array of windows, 3-letter
extensions to be checked.
References Dakota::get_pathext(), and WorkdirHelper::po_which().
Referenced by NIDRProblemDescDB::check_driver().

void split_wildcard ( const std::string & path_with_wc, bfs::path & search_dir, bfs::path & wildcard )
[static]
given a string with an optional path and a wildcard, e.g., /tmp/D*?pp, parse it into the search path /tmp (default .)
and the wildcard D*.?pp. Return wildcard as path to reduce wstring conversions
Input: path_with_wc; Output: search_dir, wildcard
Referenced by WorkdirHelper::file_op_items().

bool create_directory ( const bfs::path & dir_path, short mkdir_option ) [static]
Create a directory, with options for remove or error.
mkdir_option is DIR_CLEAN (remove and recreate), DIR_PERSIST (leave existing), or DIR_ERROR (don’t allow existing) returns whether a new directory was created.
References Dakota::abort_handler(), and WorkdirHelper::recursive_remove().
Referenced by ProcessApplicInterface::define_filenames().

void link_items ( const StringArray & source_items, const bfs::path & dest_dir, bool overwrite ) [static]
top-level link a list of source_paths (files, directories, symlinks), potentially including wildcards, from destination-
dir, which must exist
Iterate source items (paths or wildcards), linking each of them from the destination. If overwrite, remove and
replace any existing destination target, otherwise, allow to persist
References WorkdirHelper::file_op_items(), and WorkdirHelper::link().
Referenced by ProcessApplicInterface::define_filenames().

void copy_items ( const StringArray & source_items, const bfs::path & dest_dir, bool overwrite ) [static]
copy a list of source_paths (files, directories, symlinks), potentially including wildcards into destination_dir, which
must exist
Iterate source items (paths or wildcards), copying each of them into the destination. If overwrite, remove and replace any existing destination target, otherwise, allow to persist.

References WorkdirHelper::file_op_items(), and WorkdirHelper::recursive_copy().

Referenced by ProcessApplicInterface::define_filenames().

```cpp
bool link ( const bfs::path & src_path, const bfs::path & dest_dir, bool overwrite ) [static]
```

create link from dest_dir/src_path.filename() to a single path (file, dir, link) in source directory.

Assumes source file exists since it was iterated in the calling context. If overwrite, any existing file in dest_dir will be removed prior to creating the new link.

References Dakota::abort_handler().

Referenced by WorkdirHelper::link_items().

```cpp
bool recursive_copy ( const bfs::path & src_path, const bfs::path & dest_dir, bool overwrite ) [static]
```

Recursive copy of src_path into dest_dir, with optional top-level overwrite (remove/recreate) of dest_dir/src_path.filename().

Note dest_dir is the containing folder for the src_path contents to be placed in for consistency with other convenience functions (may need to reconsider).

References Dakota::abort_handler().

Referenced by WorkdirHelper::copy_items().

```cpp
bool prepend_path_item ( const bfs::path & src_path, const bfs::path & dest_dir, bool overwrite ) [static]
```

prepend the preferred env path with source path if it’s a directory; this will update cached preferred path and manipulate PATH.

prepend the env path with source path if it’s a directory or directory symlink.

References Dakota::abort_handler(), and WorkdirHelper::prepend_preferred_env_path().

Referenced by WorkdirHelper::prepend_path_items().

```cpp
bool file_op_items ( const file_op_function & file_op, const StringArray & source_items, const bfs::path & dest_dir, bool overwrite ) [static]
```

recursively perform file_op (copy, path adjust, etc.) on a list of source_paths (files, directories, symlinks), which potentially include wildcards, w.r.t. destination dir.

Iterator implementation for copy, link, etc file operation. Iterate source items (paths or wildcards), performing file_op on each w.r.t. destination. If overwrite, remove and replace any existing destination target (at top-level), otherwise, allow to persist. Return code true indicates abnormal behavior.

References WorkdirHelper::splitWildcard(), and Dakota::strContains().

Referenced by WorkdirHelper::check_equivalent_dest(), WorkdirHelper::copy_items(), WorkdirHelper::find_driver(), WorkdirHelper::link_items(), and WorkdirHelper::prepend_path_items().

```cpp
void set_preferred_path ( const boost::filesystem::path & extra_path ) [static]
```

set PATH to absolute(extra_path):dakPreferredEnvPath, without changing cached preferred PATH.

If needed, convert the passed item to an absolute path (while could make sense to prepend a relative path, no current use cases) and prepend when setting environment. Does not update cached preferred path.

References WorkdirHelper::dakPreferredEnvPath, WorkdirHelper::rel_to_abs(), and WorkdirHelper::set_environment().
bfs::path po_which ( const std::string & driver_name ) [static], [private]

Returns the bfs::path for the analysis driver - POSIX-style implementation, returns empty if not found.
  For absolute driver_name, validates that is regular file. For relative, uses string representing $PATH (preferred path) to locate an analysis driver on the host computer. Returns the path to the driver, or empty if not found.
  This is the "plain ol' which" impl that worked well, historically, on POSIX.
  References Dakota::contains(), WorkdirHelper::dakPreferredEnvPath, and WorkdirHelper::tokenize_env_path().
  Referenced by WorkdirHelper::po_which().

std::string init_startup_path ( ) [static], [private]

Initializes class member, startupPATH.
  Gets the $PATH (PATH% on windows) and returns the std::string value
  References Dakota::abort_handler().
  Referenced by WorkdirHelper::initialize().

std::string init_preferred_env_path ( ) [static], [private]

Initializes class member, dakPreferredEnvPath.
  Prepends '.' and the startupPWD to the initial startup $PATH string so that analysis driver detection is more robust
  References WorkdirHelper::startupPATH, and WorkdirHelper::startupPWD.
  Referenced by WorkdirHelper::initialize().

std::vector< std::string > tokenize_env_path ( const std::string & env_path ) [static], [private]

Tokenizes $PATH environment variable into a "list" of directories.
  Creates a a vector of directories (as an aid to search) by breaking up the $PATH environment variable (passed in as a string argument)
  Referenced by WorkdirHelper::po_which().
  The documentation for this class was generated from the following files:

  * WorkdirHelper.hpp
  * WorkdirHelper.cpp
Chapter 14

File Documentation

14.1 dakota_dll_api.cpp File Reference

This file contains a DakotaRunner class, which launches DAKOTA.

Namespaces

- Dakota
  
  *The primary namespace for DAKOTA.*

Constant Groups

- Dakota
  
  *The primary namespace for DAKOTA.*

Functions

- void DAKOTA_DLL_FN dakota_create (int *dakota_ptr_int, const char *logname)
  
  *create and configure a new DakotaRunner, adding it to list of instances*

- int DAKOTA_DLL_FN dakota_readInput (int id, const char *dakotaInput)
  
  *command DakotaRunner instance id to read from file dakotaInput*

- void DAKOTA_DLL_FN dakota_get_variable_info (int id, char **pVarNames, int *pNumVarNames, char ***pRespNames, int *pNumRespNames)
  
  *return the variable and response names*

- int DAKOTA_DLL_FN dakota_start (int id)
  
  *command DakotaRunner instance id to start (plugin interface and run strategy)*

- void DAKOTA_DLL_FN dakota_destroy (int id)
  
  *delete Dakota runner instance id and remove from active list*

- void DAKOTA_DLL_FN dakota_stop (int *id)
  
  *command DakotaRunner instance id to stop execution*

- const char *DAKOTA_DLL_FN dakota_getStatus (int id)
  
  *return current results output as a string*

- int get_mc_ptr_int ()
14.1.1 Detailed Description

This file contains a DakotaRunner class, which launches DAKOTA.

14.1.2 Function Documentation

void DAKOTA_DLL_FN dakota_stop ( int * id )
command DakotaRunner instance id to stop execution
    TODO: trick application to quit through the syscall interface or throw exception.

14.2 dakota_dll_api.h File Reference

API for DLL interactions.

Functions

- void DAKOTA_DLL_FN dakota_create ( int *dakota_ptr_int, const char *logname)
    create and configure a new DakotaRunner, adding it to list of instances
- int DAKOTA_DLL_FN dakota_readInput ( int id, const char *dakotaInput)
    command DakotaRunner instance id to read from file dakotaInput
- int DAKOTA_DLL_FN dakota_start ( int id)
    command DakotaRunner instance id to start (plugin interface and run strategy)
- void DAKOTA_DLL_FN dakota_destroy ( int id)
    delete Dakota runner instance id and remove from active list
- void DAKOTA_DLL_FN dakota_stop ( int *id)
    command DakotaRunner instance id to stop execution
- const char *DAKOTA_DLL_FN dakota_getStatus ( int id)
    return current results output as a string
- int DAKOTA_DLL_FN get_mc_ptr_int ()
    get the DAKOTA pointer to ModelCenter
- void DAKOTA_DLL_FN set_mc_ptr_int ( int ptr_int)
    set the DAKOTA pointer to ModelCenter
- int DAKOTA_DLL_FN get_dc_ptr_int ()
    get the DAKOTA pointer to ModelCenter current design point
- void DAKOTA_DLL_FN set_dc_ptr_int ( int ptr_int)
    set the DAKOTA pointer to ModelCenter current design point
14.3. DAKOTA_LINEAR_ALGEBRA.HPP FILE REFERENCE

- void DAKOTA_DLL_FN dakota_get_variable_info (int id, char ***pVarNames, int *pNumVarNames, char ***pRespNames, int *pNumRespNames)
  return the variable and response names

14.2.1 Detailed Description

API for DLL interactions.

14.2.2 Function Documentation

void DAKOTA_DLL_FN dakota_stop ( int *id )

command DakotaRunner instance id to stop execution
  TODO: trick application to quit through the syscall interface or throw exception.

14.3 dakota_linear_algebra.hpp File Reference

Dakota linear algebra utilities.

Namespaces

- Dakota
  The primary namespace for DAKOTA.

Constant Groups

- Dakota
  The primary namespace for DAKOTA.

Functions

- void svd (RealMatrix &matrix, RealVector &singular_vals, RealMatrix &v_trans, bool compute_vectors=true)
  Compute the SVD of an arbitrary matrix \( A = USV^T \).

- void singular_values (RealMatrix &matrix, RealVector &singular_values)
  compute the singular values without storing any singular vectors (A will be destroyed)

- int qr (RealMatrix &A)
  Compute an in-place QR factorization \( A = QR \).

- int qr_rsolve (const RealMatrix &q,r, bool transpose, RealMatrix &rhs)
  Perform a multiple right-hand sides \( Rinv \ast rhs \) solve using the \( R \) from a qr factorization.

- double det_AtransA (RealMatrix &A)
  Use SVD to compute \( \text{det}(A' \ast A) \), destroying A with the SVD.

14.3.1 Detailed Description

Dakota linear algebra utilities. Convenience functions to perform Teuchos::LAPACK operations on Dakota RealMatrix/RealVector.
14.4 dakota_tabular_io.hpp File Reference

Utility functions for reading and writing tabular data files. Emerging utilities for tabular file I/O. For now, just extraction of capability from separate contexts to facilitate rework. These augment (and leverage) those in data_-util.h.

Namespaces

- Dakota
  
  The primary namespace for DAKOTA.

Constant Groups

- Dakota
  
  The primary namespace for DAKOTA.

Functions

- String format_name (unsigned short tabular_format)
  
  Translate tabular_format into a user-friendly name.

- void print_expected_format (std::ostream &s, unsigned short tabular_format, size_t num_rows, size_t num_cols)
  
  Describe the expected data file format based on passed parameters.

- void print_unexpected_data (std::ostream &s, const String &filename, const String &context_message, unsigned short tabular_format)
  
  Print a warning if there's extra data in the file.

- void open_file (std::ifstream &data_file, const std::string &input_filename, const std::string &context_message)
  
  open the file specified by name for reading, using passed input stream, presenting context-specific error on failure

- void open_file (std::ofstream &data_file, const std::string &output_filename, const std::string &context_message)
  
  open the file specified by name for writing, using passed output stream, presenting context-specific error on failure

- void close_file (std::ifstream &data_file, const std::string &input_filename, const std::string &context_message)
  
  close the file specified by name after reading, using passed input stream, presenting context-specific error on failure

- void close_file (std::ofstream &data_file, const std::string &output_filename, const std::string &context_message)
  
  close the file specified by name after writing, using passed output stream, presenting context-specific error on failure

- void write_header_tabular (std::ostream &tabular_ostream, const Variables &vars, const Response &response, const std::string &counter_label, unsigned short tabular_format)
  
  Output the header row (labels) for a tabular data file for variables and responses, with variables in input spec order. Conditionally include interface ID. Primary uses: environment tabular data, pre-run output, surrogate approx evals.

- void write_header_tabular (std::ostream &tabular_ostream, const Variables &vars, const StringArray &addtnl_labels, const std::string &counter_label, unsigned short tabular_format)
Output the header row (labels) for a tabular data file for variables and additional labels not tied to a response. Variables are in input spec order. Conditionally include interface ID. Primary uses: MCMC chain export, including calibration sigmas.

- **void write_leading_columns** (std::ostream &tabular_ostream, size_t eval_id, const String &iface_id, unsigned short tabular_format)
  
  Write the leading column with eval ID and conditionally, the interface ID.

- **void write_data_tabular** (std::ostream &tabular_ostream, const Variables &vars, const String &iface, size_t counter, unsigned short tabular_format)
  
  Output a row of tabular data from a variables object. All active/inactive variables written in input spec order. Conditionally include interface ID. Primary uses: output of sampling sets.

- **void write_data_tabular** (std::ostream &tabular_ostream, const Variables &vars, const String &iface, const Response &response, size_t counter, unsigned short tabular_format)
  
  Output a row of tabular data from variables and response objects. All active/inactive variables written in input spec order. Conditionally include interface ID. Primary uses: environment tabular data, pre-run output, surrogate approx evals.

- **void write_data_tabular** (const std::string &output_filename, const std::string &context_message, const RealVectorArray &output_coeffs, const UShort2DArray &output_indices)
  
  PCE export: write freeform format file with whitespace-separated data where each row has num_fns reals from coeffs, followed by num_vars unsigned shorts from indices.

- **bool exists_extra_data** (std::istream &tabular_file)
  
  Check if an input stream contains unexpected additional data.

- **void read_header_tabular** (std::istream &input_stream, unsigned short tabular_format)
  
  read and discard header line from the stream

- **int read_leading_columns** (std::istream &input_stream, unsigned short tabular_format)
  
  read leading columns [ int eval_id [ String iface_id ] ]

- **void read_leading_columns** (std::istream &input_stream, unsigned short tabular_format, int &eval_id, String &iface_id)
  
  read leading columns [ int eval_id [ String iface_id ] ]

- **void read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealVector &input_data, size_t num_entries, unsigned short tabular_format)
  
  read possibly header-annotated whitespace-separated data into a vector of length num_entries; if annotated then it's a column vector for now

- **void read_data_tabular** (const std::string &input_filename, const std::string &context_message, const Variables &vars, size_t num_fns, RealMatrix &vars_matrix, RealMatrix &resp_matrix, unsigned short tabular_format, bool active_only)
  
  Tabular read for ApproximationInterface challenge data: read possibly header-annotated whitespace-separated data of possible mixed Variables, followed by num_fns, each into RealMatrix with minimal error checking.

- **void read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealVectorArray &input_coeffs, UShort2DArray &input_indices, unsigned short tabular_format, size_t num_vars, size_t num_fns)
  
  Tabular read for PCE import: read possibly header-annotated whitespace-separated data of unknown length where each row has num_fns reals followed by num_vars unsigned shorts; append data to arrays passed by reference.

- **void read_data_tabular** (const std::string &input_filename, const std::string &context_message, Variables &vars, Response &resp, PRPList &input_prp, unsigned short tabular_format, bool verbose=false, bool active_only=false)
  
  Tabular read for DataFitSurrModel (build points): read whitespace-separated data with optional row and column headers into lists of Variables and Responses until out of data.
void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealMatrix &input_matrix, size_t record_len, unsigned short tabular_format, bool verbose=false)

Tabular read for import_approx_points_file: read whitespace-separated data with optional row and column headers into a single matrix, with length of record as specified and number of records to be determined by file content. The matrix is stored as record_len rows by num_records columns.

void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealMatrix &input_matrix, size_t num_rows, size_t num_cols, unsigned short tabular_format, bool verbose=false)

Tabular read for GPMSA data: read whitespace-separated data with optional row and column headers into a single matrix, with size as specified (one experiment per row).

size_t **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealVectorArray &cva, IntVectorArray &diva, StringMulti2DArray &dsva, RealVectorArray &drva, unsigned short tabular_format, bool active_only, Variables vars)

Tabular read for ParamStudy: read specified input data file into arrays with sizes specified by the passed vc_totals array.

### 14.4.1 Detailed Description

Utility functions for reading and writing tabular data files. Emerging utilities for tabular file I/O. For now, just extraction of capability from separate contexts to facilitate rework. These augment (and leverage) those in data-util.h. Design/capability goals: Ability to read / write data with row/col headers or in free-form Detect premature end of file, report if extra data. More consistent and reliable checks for file open errors. Require right number of cols in header mode; only total data checking in free-form (likely) Allow comment character for header rows or even in data? variables vs. variables/responses for both read and write. Should we support CSV? delimiter = ','; other? Verify treatment of trailing newline without reading a zero. Allow reading into the transpose of the data structure.

### 14.5 dll_tester.cpp File Reference

Test the DLL with a DAKOTA input file.

**Functions**

- int **main** (int argc, char ∗argv[ ])

  The main program for exercising the DLL API with a simple command-line.

### 14.5.1 Detailed Description

Test the DLL with a DAKOTA input file.

### 14.6 JEGAOptimizer.cpp File Reference

Contains the implementation of the JEGAOptimizer class.

**Classes**

- class **JEGAOptimizer::Evaluator**

  An evaluator specialization that knows how to interact with Dakota.
• class JEGAOptimizer::EvaluatorCreator
  A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.
• class JEGAOptimizer::Driver
  A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.

Namespaces
• Dakota
  The primary namespace for DAKOTA.

Constant Groups
• Dakota
  The primary namespace for DAKOTA.

Functions
• template<typename T>
  string asstring (const T &val)
  Creates a string from the argument val using an ostringstream.

14.6.1 Detailed Description
Contains the implementation of the JEGAOptimizer class.

14.7 JEGAOptimizer.hpp File Reference
Contains the definition of the JEGAOptimizer class.

Classes
• class JEGAOptimizer
  A version of Dakota::Optimizer for instantiation of John Eddy’s Genetic Algorithms (JEGA).

Namespaces
• Dakota
  The primary namespace for DAKOTA.

Constant Groups
• Dakota
  The primary namespace for DAKOTA.

14.7.1 Detailed Description
Contains the definition of the JEGAOptimizer class.
14.8 library_mode.cpp File Reference

file containing a mock simulator main for testing Dakota in library mode

Classes

- struct callback_data

Functions

- void fpinit_AS ()
- void run_dakota_parse (const char *dakota_input_file)
  
  Run a Dakota LibraryEnvironment, mode 1: parsing an input file.
- void run_dakota_data ()
  
  Run a Dakota LibraryEnvironment, mode 2: from C++ API inserted data.
- void run_dakota_mixed (const char *dakota_input_file, bool mpirun_flag)
  
  Run a Dakota LibraryEnvironment, from string or input file input, supplemented with additional C++ API adjustments.
- void serial_interface_plugin (Dakota::LibraryEnvironment &env)
  
  Convenience function with simplest example of interface plugin: plugin a serial DirectApplicInterface that can be constructed independent of Dakota’s configuration details.
- void parallel_interface_plugin (Dakota::LibraryEnvironment &env)
  
  Convenience function to plug a library client’s interface into the appropriate model, demonstrating use of Dakota parallel configuration in constructing the plugin Interface on the right MPI_Comm.
- static void callback_function (Dakota::ProblemDescDB *db, void *ptr)
  
  Example: user-provided post-parse callback (Dakota::DbCallbackFunction)
- int main (int argc, char *argv[])
  
  A mock simulator main for testing Dakota in library mode.

Variables

- static const char serial_input []
  
  Default Dakota input string for serial case (rosenbrock):
- static const char parallel_input []
  
  Default Dakota input string for parallel case (text_book)

14.8.1 Detailed Description

file containing a mock simulator main for testing Dakota in library mode

14.8.2 Function Documentation

void fpinit_AS ()

Floating-point initialization from AMPL: switch to 53-bit rounding if appropriate, to eliminate some cross-platform differences.

  Referenced by main().
void run_dakota_parse ( const char * dakota_input_file )

Run a Dakota LibraryEnvironment, mode 1: parsing an input file.

Simplest library case: this function parses from an input file to define the ProblemDescDB data.
References Environment::execute(), ProgramOptions::input_file(), Environment::mpi_manager(), MPIManager::mpi_run_flag(), parallel_interface_plugin(), serial_interface_plugin(), and MPIManager::world_rank().

Referenced by run_dakota_data().

void run_dakota_data ( )

Run a Dakota LibraryEnvironment, mode 2: from C++ API inserted data.

Rather than parsing from an input file, this function populates Data class objects directly using a minimal specification and relies on constructor defaults and post-processing in post_process() to fill in the rest.
References DataInterface::data_rep(), DataResponses::data_rep(), DataVariables::data_rep(), DataMethod::data_rep(), LibraryEnvironment::done_modifying_db(), Environment::execute(), Environment::exit_mode(), DataResponsesRep::gradientType, DataResponsesRep::hessianType, LibraryEnvironment::insert_nodes(), DataMethodRep::methodName, Environment::mpi_manager(), MPIManager::mpi_run_flag(), ParallelLibrary::mpi_run_flag(), DataVariablesRep::numContinuousDesVars, DataResponsesRep::numNonlinearIneqConstraints, DataResponsesRep::numObjectiveFunctions, parallel_interface_plugin(), Environment::parallel_library(), serial_interface_plugin(), and ParallelLibrary::world_rank().

Referenced by run_dakota_parse().

void run_dakota_mixed ( const char * dakota_input_file, bool mpirun_flag )

Run a Dakota LibraryEnvironment, from string or input file input, supplemented with additional C++ API adjustments.

Function to encapsulate the Dakota object instantiations for mode 3: mixed parsing and direct updating.

This function showcases multiple features. For parsing, either an input file (dakota_input_file != NULL) or a default input string (dakota_input_file == NULL) are shown. This parsed input is then mixed with input from three sources: (1) input from a user-supplied callback function, (2) updates to the DB prior to Environment instantiation, (3) updates directly to Iterators/Models following Environment instantiation.

References callback_function(), LibraryEnvironment::done_modifying_db(), ProgramOptions::echo_input(), Environment::execute(), LibraryEnvironment::filtered_model_list(), ProblemDescDB::get_sa(), ProgramOptions::input_file(), ProgramOptions::input_string(), Environment::mpi_manager(), MPIManager::mpi_run_flag(), parallel_input, parallel_interface_plugin(), Environment::parallel_library(), Environment::problem_description_db(), ProblemDescDB::resolve_top_method(), callback_data::rosen_cdv_upper_bd, serial_input, serial_interface_plugin(), ProblemDescDB::set(), and ParallelLibrary::world_rank().

Referenced by run_dakota_data().

void serial_interface_plugin ( Dakota::LibraryEnvironment & env )

Convenience function with simplest example of interface plugin: plugin a serial DirectApplicInterface that can be constructed independent of Dakota’s configuration details.

Demonstration of simple plugin where client code doesn’t require access to detailed Dakota data (such as Model-based parallel configuration information) to construct the DirectApplicInterface. This example plugs-in a derived serial direct application interface instance ("plugin_rosenbrock").

References Dakota::abort_handler(), LibraryEnvironment::plugin_interface(), and Environment::problem_description_db().

Referenced by run_dakota_data(), run_dakota_mixed(), and run_dakota_parse().
CHAPTER 14. FILE DOCUMENTATION

void parallel_interface_plugin ( Dakota::LibraryEnvironment & env )

Convenience function to plug a library client’s interface into the appropriate model, demonstrating use of Dakota parallel configuration in constructing the plugin Interface on the right MPI Comm.

From a filtered list of Model candidates, plug-in a derived direct application interface instance ("plugin_textbook" for parallel). This approach provides more complete access to the Model, e.g., for access to analysis communicators.

References Dakota::abort_handler(), Interface::assign_rep(), LibraryEnvironment::filtered_model_list(), ProblemDescDB::get_db_model_node(), Environment::problem_description_db(), and ProblemDescDB::set_db_model_nodes().

Referenced by run_dakota_data(), run_dakota_mixed(), and run_dakota_parse().

static void callback_function ( Dakota::ProblemDescDB * db, void * ptr ) [static]

Example: user-provided post-parse callback (Dakota::DbCallbackFunction)

Example of user-provided callback function (an instance of Dakota::DbCallbackFunction) to override input provided by parsed Dakota input file or input string data.

References Dakota::contains(), ProblemDescDB::get_sa(), ProblemDescDB::get_ushort(), ProblemDescDB::resolve_top_method(), callback_data::rosen_cdv_upper_bd, and ProblemDescDB::set().

Referenced by run_dakota_mixed().

int main ( int argc, char * argv[] )

A mock simulator main for testing Dakota in library mode.

Overall Usage: dakota_library_mode [-mixed] [dakota.in]

Uses alternative instantiation syntax as described in the library mode documentation within the Developers Manual. Tests several problem specification modes:

(1) run_dakota_parse: reads all problem specification data from a Dakota input file. Usage: dakota_library_mode dakota.in

(2) run_dakota_data: creates all problem specification from direct Data instance instantiations in the C++ code. Usage: dakota_library_mode

(3) run_dakota_mixed: a mixture of input parsing and direct data updates, where the data updates occur: (a) via the DB during Environment instantiation, and (b) via Iterators/Models following Environment instantiation. Usage: dakota_library_mode -mixed (input from default string) dakota_library_mode -mixed dakota.in (input from specified file)

Serial cases use a plugin rosenbrock model, while parallel cases use textbook.

References MPIManager::detect_parallel_launch(), fpinit_ASL(), Dakota::mpi_debug_hold(), run_dakota_data(), run_dakota_mixed(), and run_dakota_parse().

14.8.3 Variable Documentation

const char serial_input[] [static]

Initial value:

" method,"
" optpp q newton"
" max_iterations = 50"
" convergence_tolerance = 1e-4"
" variables,"
" continuous_design = 2"
" descriptors 'x1' 'x2'
" interface,"
" direct"
" analysis_driver = 'plugin_rosenbrock'"
Default Dakota input string for serial case (rosenbrock):
Referenced by run_dakota_mixed().

```
const char parallel_input[ ] [static]

Initial value:
```

Default Dakota input string for parallel case (text_book)
Referenced by run_dakota_mixed().

14.9 library_split.cpp File Reference

file containing a mock simulator main for testing DAKOTA in library mode on a split communicator

Functions

- void manage_mpi (MPI_Comm &my_comm, int &color)
  
  *Split MPI_COMM_WORLD, returning the comm and color.*

- void gen_dakota_input (const int &color, std::string &input)
  
  *Return the appropriate DAKOTA input based on color (1 or 2)*

- void run_dakota (const MPI_Comm &comm, const std::string &input, const int &color)
  
  *Launch DAKOTA on passed communicator, tagging output/error with color.*

- void collect_results ()
  
  *Wait for and collect results from DAKOTA runs.*

- int main (int argc, char *argv[ ])
  
  *Driver routine for testing library mode with partitioned MPI_Comm. This test fixture requires MPI and can be run on 3–8 processors.*

14.9.1 Detailed Description

file containing a mock simulator main for testing DAKOTA in library mode on a split communicator
14.10 main.cpp File Reference

file containing the main program for DAKOTA

Functions

- void fpinit ASL()
- int main(int argc, char *argv[])

The main DAKOTA program.

14.10.1 Detailed Description

file containing the main program for DAKOTA

14.10.2 Function Documentation

void fpinit ASL()

Floating-point initialization from AMPL: switch to 53-bit rounding if appropriate, to eliminate some cross-platform differences.

int main(int argc, char *argv[])

The main DAKOTA program.

Manage command line inputs, input files, restart file(s), output streams, and top level parallel iterator communicators. Instantiate the ExecutableEnvironment and invoke its execute() virtual function.

References Environment::check(), ExecutableEnvironment::execute(), fpinit ASL(), Dakota::mpi_debug_hold(), and Dakota::register_signal_handlers().

14.11 restart_util.cpp File Reference

file containing the DAKOTA restart utility main program

Namespaces

- Dakota

  The primary namespace for DAKOTA.

Constant Groups

- Dakota

  The primary namespace for DAKOTA.
14.11. RESTART_UTIL.CPP FILE REFERENCE

Functions

- void print_usage (std::ostream &s)
  
  print restart utility help message
- void print_restart (StringArray pos_args, String print_dest)
  
  print a restart file
- void print_restart pdb (StringArray pos_args, String print_dest)
  
  print a restart file (PDB format)
- void print_restart_tabular (StringArray pos_args, String print_dest, unsigned short tabular_format, int tabular_precision)
  
  print a restart file (tabular format)
- void read_neutral (StringArray pos_args)
  
  read a restart file (neutral file format)
- void repair_restart (StringArray pos_args, String identifier_type)
  
  repair a restart file by removing corrupted evaluations
- void concatenate_restart (StringArray pos_args)
  
  concatenate multiple restart files
- int main (int argc, char *argv[])
  
  The main program for the DAKOTA restart utility.

14.11.1 Detailed Description

file containing the DAKOTA restart utility main program

14.11.2 Function Documentation

int main ( int argc, char * argv[] )

The main program for the DAKOTA restart utility.

  Parse command line inputs and invoke the appropriate utility function (print_restart(), print_restart_tabular(), read_neutral(), repair_restart(), or concatenate_restart()).

  References Dakota::concatenate_restart(), Dakota::print_restart(), Dakota::print_restart_pdb(), Dakota::print_restart_tabular(), Dakota::print_usage(), Dakota::read_neutral(), Dakota::repair_restart(), and Dakota::write_precision.
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