DAKOTA Integration

http://dakota.sandia.gov

- **Class-selected getting started or advanced usage topics**
- **How DAKOTA interfaces with a simulation (computational model)**
- **Steps in building a black-box interface script:**
  - **Integrate parameters from DAKOTA (aprepro/dprepro)**
  - **Run analysis**
  - **Post-process to capture results of interest**
- **Build interface to your code and then share your experience**

Training materials can be viewed at:
http://dakota.sandia.gov/training/2011

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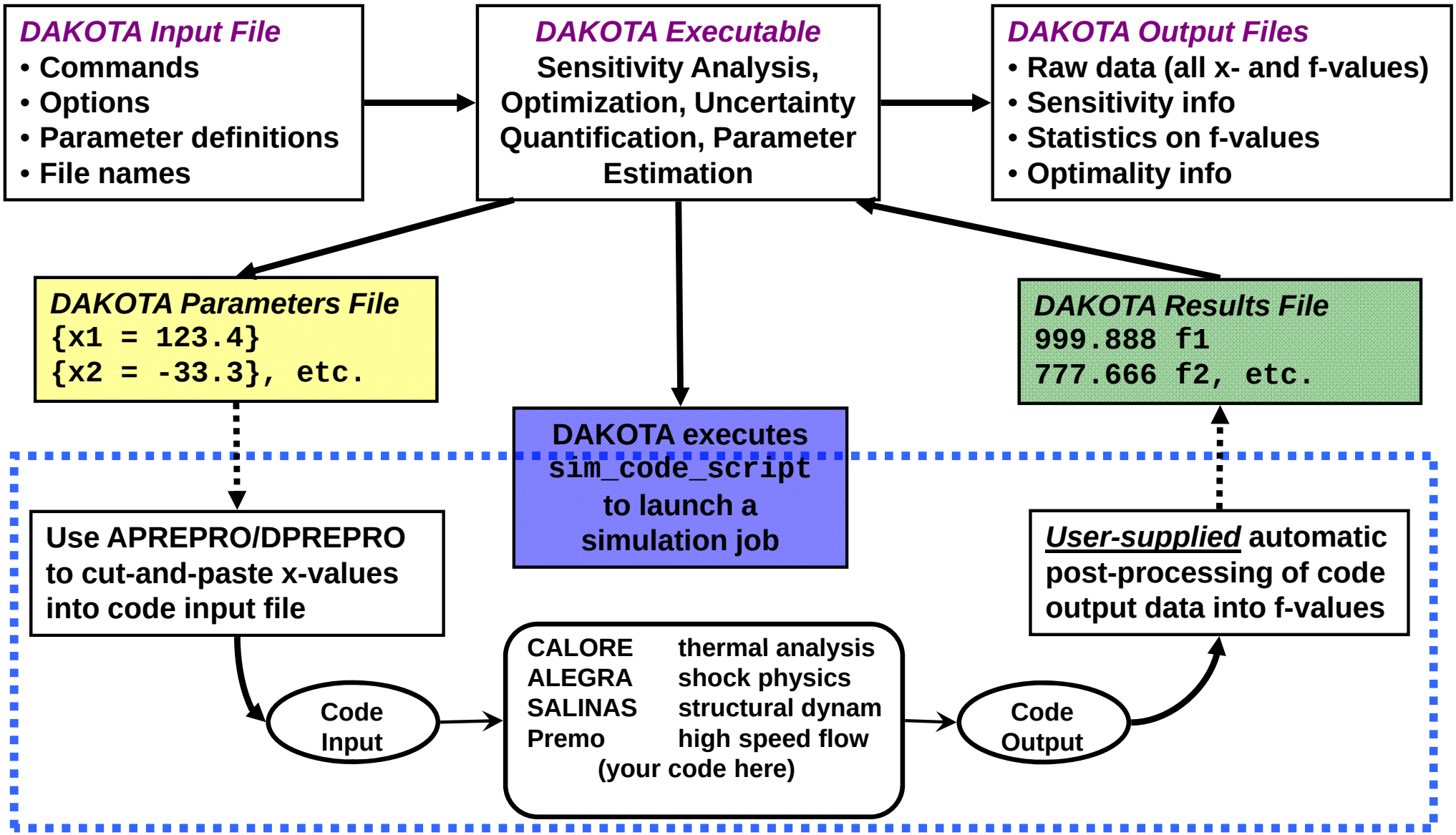
DAKOTA Execution & Info Flow



DAKOTA Application Interfacing Class

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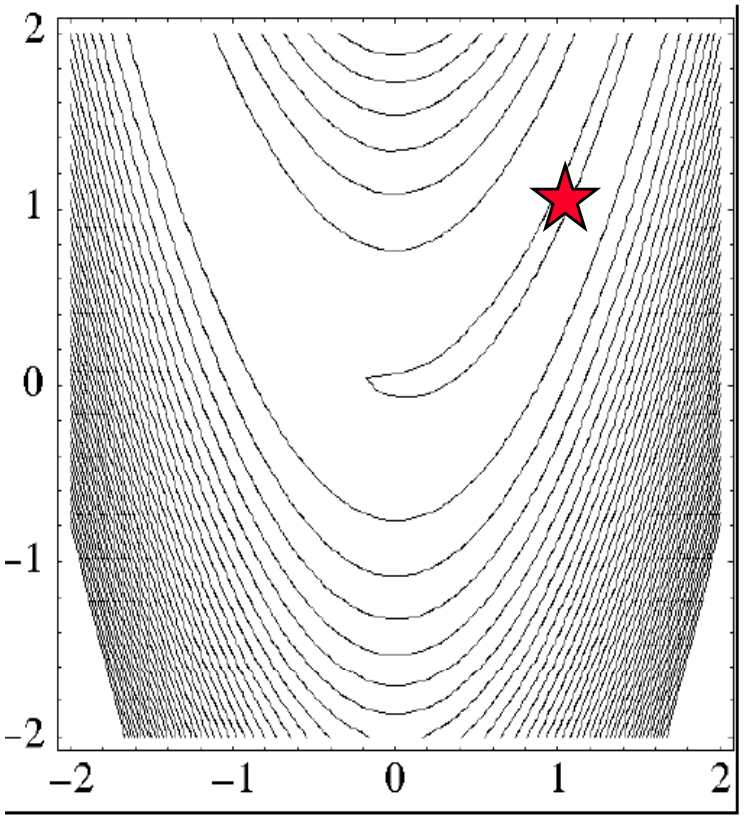
Application Stand-in: Rosenbrock "Banana" Function

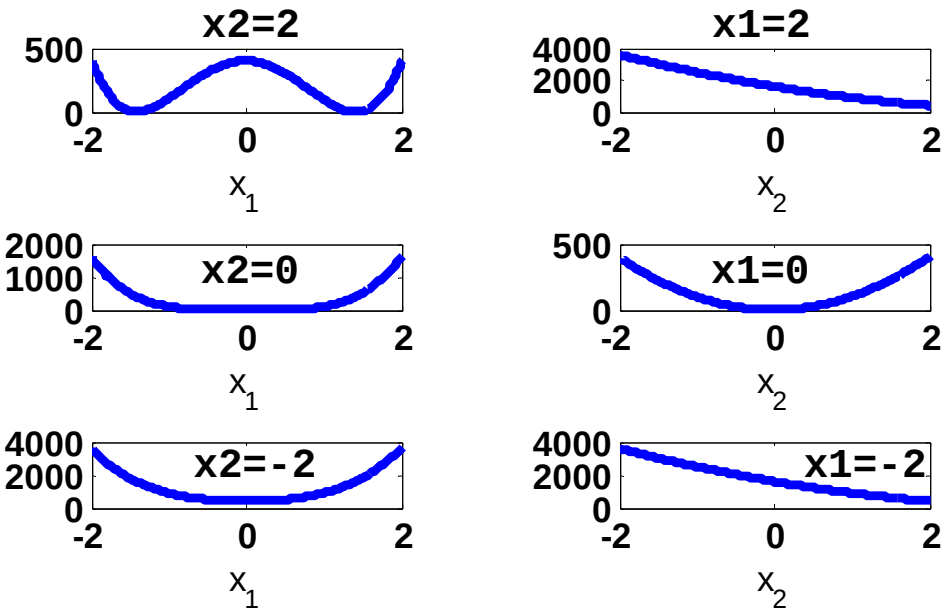
$f(x1,x2) = 100*(x2-x1*x1)^2 + (1-x1)^2$

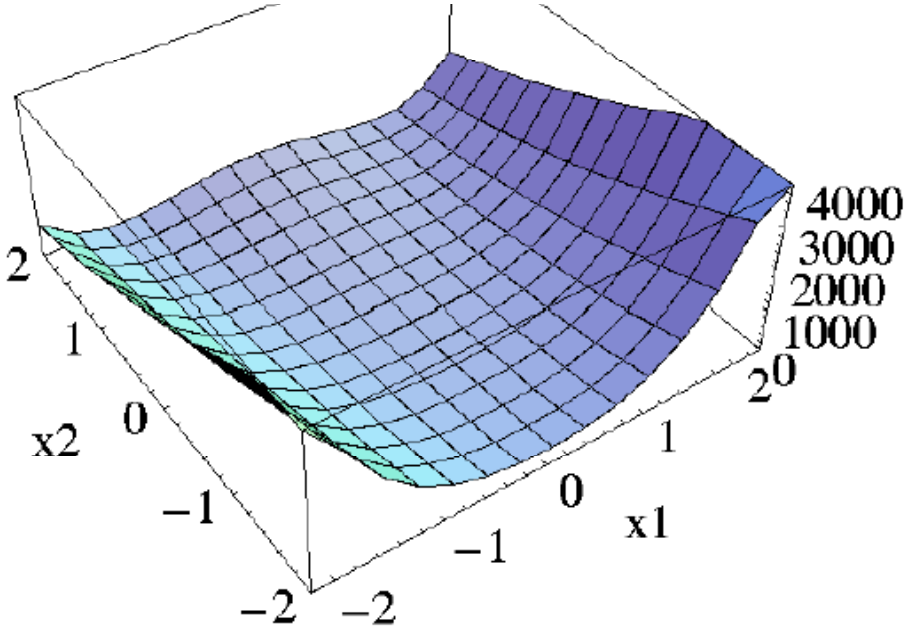
$-2 \leq x1 \leq 2$

$-2 \leq x2 \leq 2$

Minimum: $f(x1,x2) = f(1,1) = 0.0$







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Demo:
Rosenbrock as a “black box”

- Locate example in `Dakota/examples/script_interfaces/generic`
- Described in DAKOTA 5.1 User’s Manual 17.1
- Explore top-down (DAKOTA down to application and back)
- Since you’re familiar with your application, may want to build from application up

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Interfacing to Your Simulation (Assuming Text-based I/O)

1. Annotate your input file to create template
   `{ stress }` `{ alpha1 }`
2. Create a representative DAKOTA `params.in` file in aprepro format (see User's 12.6.2) and test:
   `dprepro params.in analysis.in.template analysis.in`
3. Verify commands to run application with `analysis.in`
4. Determine how to automatically extract results of interest (direct application to export, shell commands, python, perl, visual basic, etc.) to create `results.out` (see User's 14.2)
5. Assemble into a script, e.g., `run_analysis.sh`; test script with sample params.in:
   `./run_analysis.sh params.in results.out`
6. Test with a simple DAKOTA input deck, e.g., parameter study

Method Summary

Time-tested and advanced algorithms for deterministic and probabilistic analysis in a single toolkit to address simulations that are: nonsmooth, discontinuous, multimodal, expensive, mixed variable, failure-prone

Gradient-based Optimization

- **DOT: frcg, bfgs, mmfd, slp, sqp**
- **CONMIN: frcg, mfd**
- **NPSOL sqp**
- **NLPQLP sqp**
- **OPT++: prcg, QN NIP, FDN NIP, FN NIP**
- **Dynamic plug-in: SNOPT, …**

Derivative-free Optimization

- **COLINY: PS, EA, Solis-Wets, COBYLA, DIRECT**
- **JEGA: MOGA, SOGA**
- **NCSU: DIRECT, IFFCO**
- **OPT++: PDS**
- **APPSPACK, EGO, TMF**

Parameter estimation (calibration)

- **Nonlinear least squares: NL2SOL, NLSSOL, OPT++ Gauss-Newton**

Sensitivity/statistical analysis

- **Parameter studies: vector, list, centered, grid**
- **Design of experiments:**
  - **DDACE: LHS, MC, grid, OA, OA_LHS, CCD, BB**
  - **FSUDace: CVT, Halton, Hammersley**
  - **PSUADE: MOAT**

Uncertainty quantification

- **Sampling: LHS, MC, Incr. LHS, IS/AIS/MMAIS**
- **Local Reliability: MVFOSM/MVSOSM, x/u AMV/AMV^2, x/u AMV+/AMV^2+, x/u TANA, FORM/SORM**
- **Global Reliability: EGRA**
- **Stochastic expansions: Wiener-Askey gen. Polynomial Chaos (Hermite, Legendre, Laguerre, Jacobi, gen. Laguerre); Stochastic collocation (Lagrange)**
- **Epistemic: Second-order probability, Dempster Shafer Theory of Evidence**

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Advanced Topics (dictated by class interest)

General features

- Restart
- Evaluation cache
- Utilities in dakota_restart_util
- Tabular graphics data
- Failure capturing: abort, retry, recover, ignore
- Constraint specification: linear, nonlinear; equality, inequality
- Input/output scaling
- Matlab interface

Approximation methods

- Global data fit surrogate methods (polynomials, MARS, Kriging, etc.)
- Local surrogate methods (Taylor series, multipoint)
- Hierarchical: high/low fidelity models
- Corrections

Strategies/Advanced approaches

- Nested models: OUU
- Multi-objective (Pareto) optimization
- Multistart; multi-level hybrid
- Surrogate-based optimization (variety of constraint handling approaches): trust region; EGO/EGRA
- Reliability-based design optimization
- Advanced UQ topics: polynomial chaos, second-order probability, Dempster-Shafer, surrogate-based UQ
- AMPL: for analytic problems / algebraic mappings

Parallel capabilities: message passing, asynchronous local, hybrid

- Asynchronous evaluations
- Dakota parallel, application serial
- Dakota serial, application parallel
- Multi-level parallel: concurrent iteration, concurrent function evaluations, concurrent analyses,
- multiprocessor simulations

Getting Started with DAKOTA

- **Access a Sandia installation: `module avail dakota`**
  AMECH (CA), CEE (ESHPC/SCICO, NM), Computer clusters (both)
  or download (see Analyst Home Page or DAKOTA webpage)

- **Supported on Linux, Solaris, AIX (purple), Mac OS X, Windows (no MinGW or Cygwin install required), Redstorm**

- **Key resource: http://dakota.sandia.gov/**
  - **Extensive documentation (user, reference, developer)**
  - **Support mailing lists / archives**
  - **Software downloads: releases and nightly stable & VOTD builds (freely available worldwide via GNU GPL)**

- **User's Manual, Chapter 2: Tutorial with example input files**

- **Support:**
  - **dakota-users@software.sandia.gov (DAKOTA team and internal/external user community)**
  - **dakota-help@sandia.gov (for SNL-specific or issues involving proprietary information)**

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