DAKOTA 101

DAKOTA Overview

http://dakota.sandia.gov/

Learning goals: Understand:

- **How DAKOTA interfaces with a simulation (computational model)**
- **DAKOTA input file structure; corresponding DAKOTA abstractions**
- **How to run DAKOTA and JAGUAR to perform parameter studies**
- **DAKOTA framework benefits**

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

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DAKOTA in a Nutshell

Design and Analysis toolKit for Optimization and Terascale Applications includes a wide array of algorithm capabilities to support engineering transformation through advanced modeling and simulation.

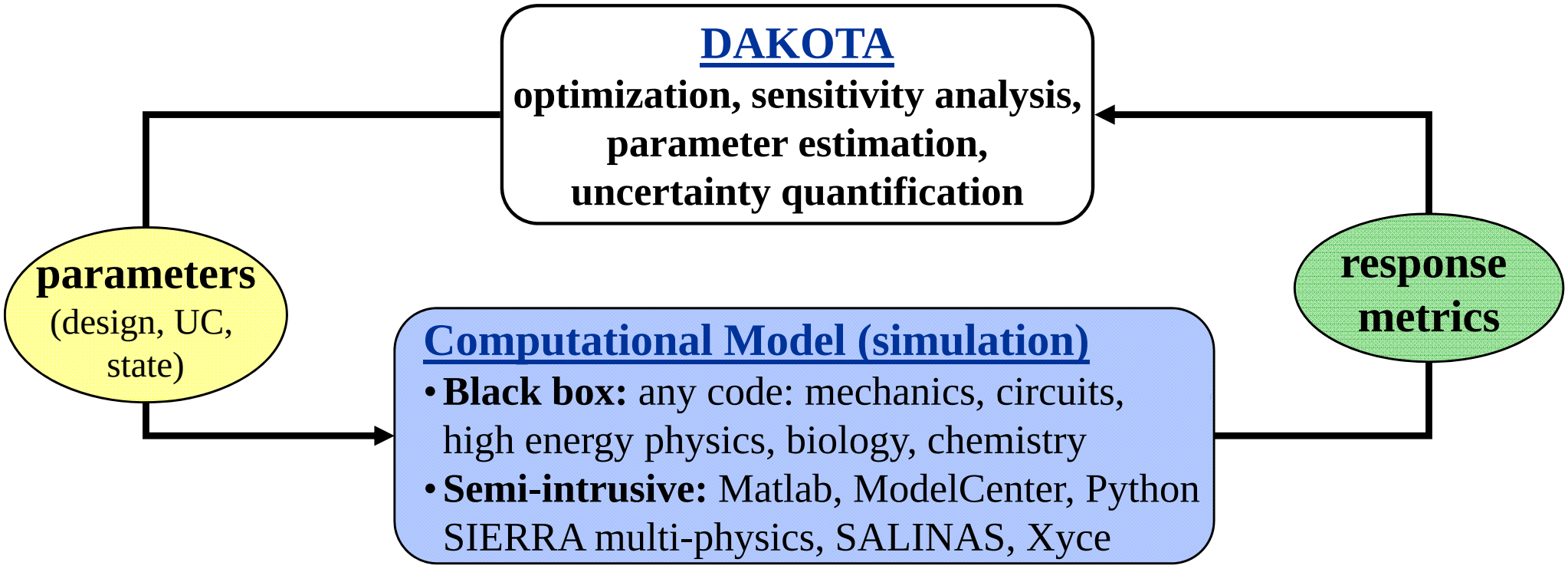
Adds value to simulation-based analysis by answering fundamental science and engineering questions:

- **What are the crucial factors/parameters and how do they affect key metrics? *(sensitivity)***
- **How safe, reliable, robust, or variable is my system? *(quantification of margins and uncertainty: QMU, UQ)***
- **What is the best performing design or control? *(optimization)***
- **What models and parameters best match experimental data? *(calibration)***

- ***All rely on iterative analysis with a computational model for the phenomenon of interest***

Automated Iterative Analysis

Automate typical "parameter variation" studies with advanced methods and a generic interface to your simulation



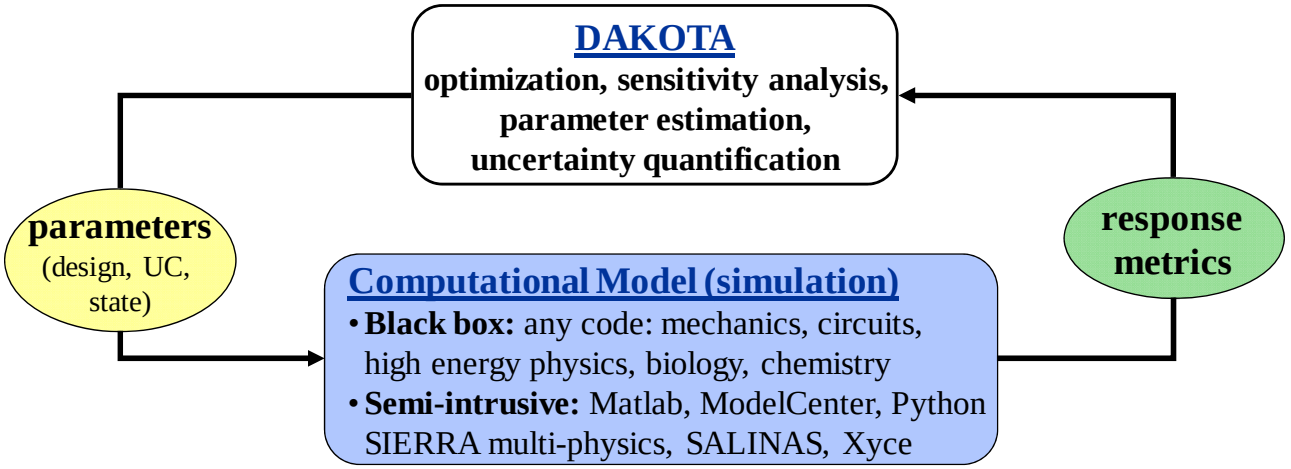
- **Can support experimental testing: examine many accident conditions with computer models, then physically test a few worst-case conditions.**

Key DAKOTA Capabilities

- **Generic interface to simulations**
- **Time-tested and advanced algorithms to address non-smooth, discontinuous, multimodal, expensive, mixed variable, failure-prone**
- **Strategies to combine methods for advanced studies or improve efficiency with surrogates (meta-models)**
- **Mixed deterministic / probabilistic analysis**
- **Supports scalable parallel computations on clusters**
- **Object-oriented code; modern software quality practices**
- **Limited Windows interface (run via command prompt); however new graphical user interface. DART integration in progress.**

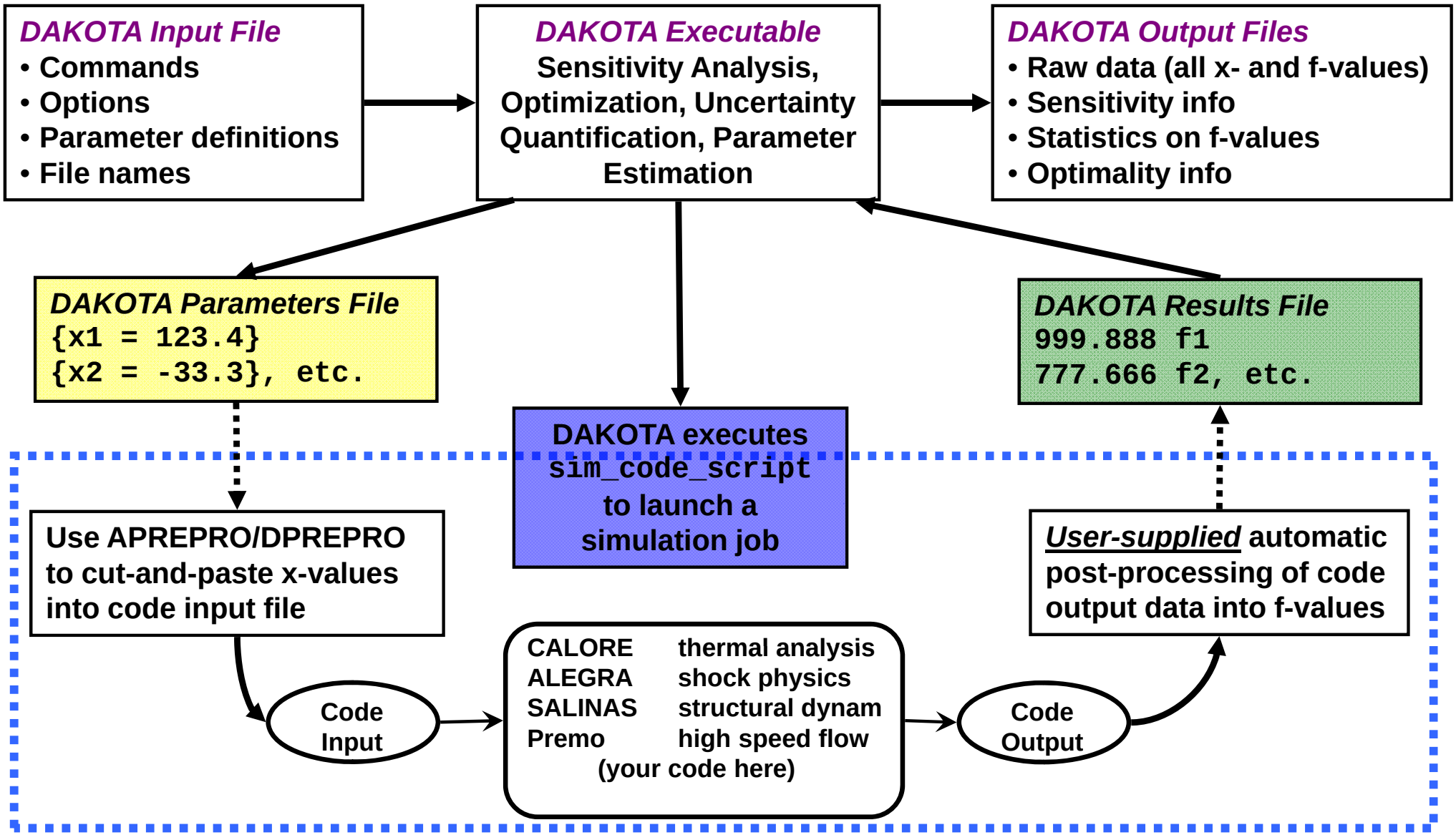
- **Additional details: http://dakota.sandia.gov/**
  - **Extensive documentation, including a tutorial**
  - **Support resources: http://dakota.sandia.gov/resources.html**
  - **Software downloads: stable releases and nightly builds (freely available worldwide via GNU LGPL)**

Overall DAKOTA 101 Goals



- **DAKOTA 101 will focus on setting up various kinds of studies to drive this iterative flow**
- **We'll use JAGUAR GUI or text file editing to create input files, with command line run**
- **For this class we'll substitute test functions from the DAKOTA distribution for the simulation**
- ***DAKOTA Integration focuses on connecting to your actual application***

DAKOTA Execution & Info Flow



DAKOTA Application Interfacing Class

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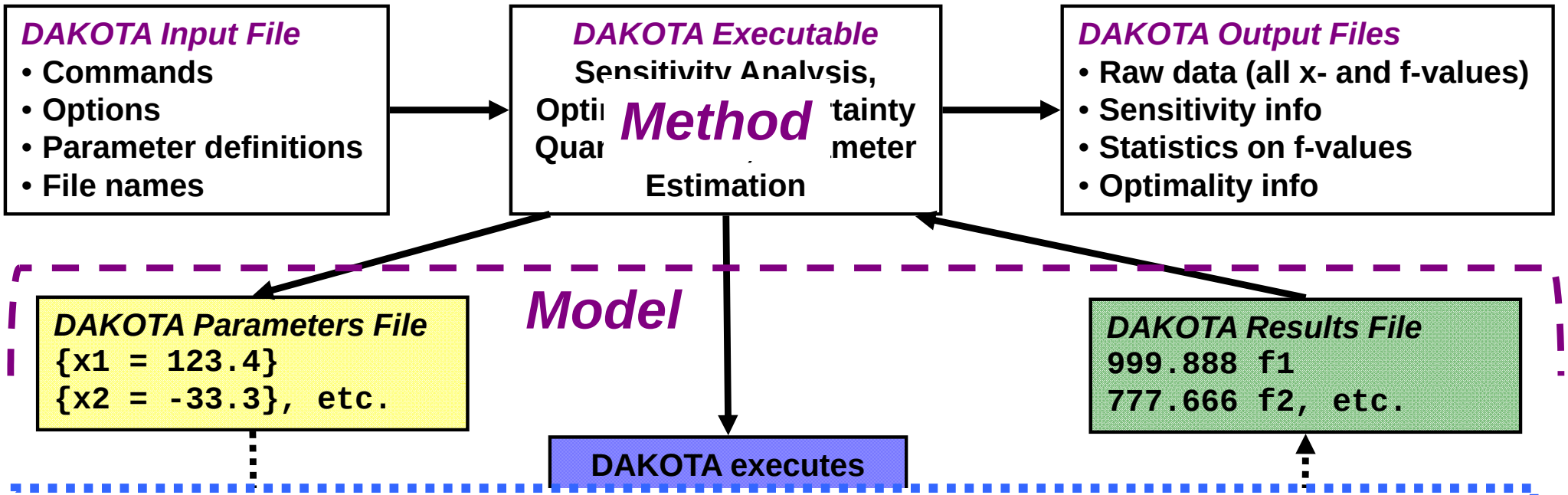
DAKOTA Execution & Info Flow



Algebraic test function which "reads" parameters and writes results, e.g.,

`rosenbrock`
`text_book`
`cantilever`

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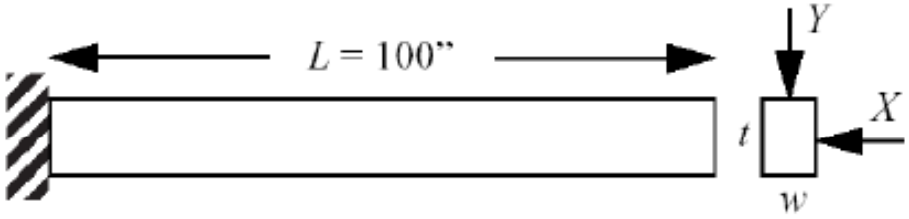
Cantilever Beam Analysis Problem



- **Design goal: minimize weight (*A=w*t*) subject to constraints**
  `1.0 ≤ beam_width ≤ 4.0, 1.0 ≤ beam_thickness ≤ 4.0,`

$$stress = \frac{600}{wt^2}Y + \frac{600}{w^2t}X \le R$$

$$displacement = \frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} \le D_0$$

Given values of *w, t, R, E, X, Y,* DAKOTA's `mod_cantilever` driver computes *area, stress-R, displacement-D_0*

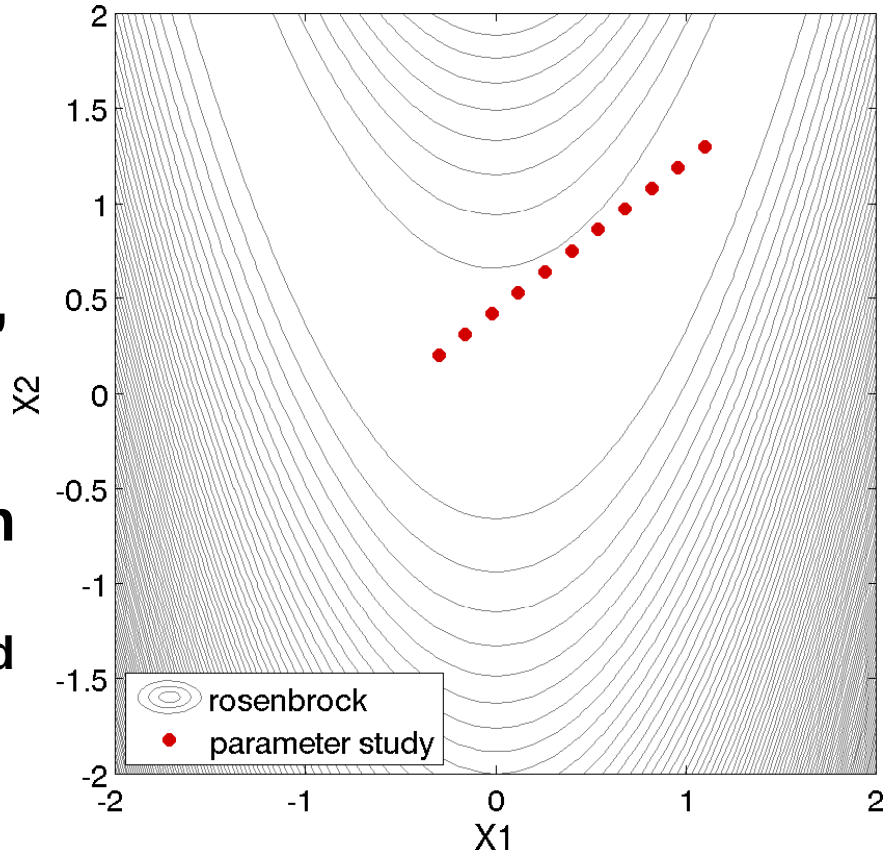
- **And potentially, subject to uncertainties:**
  - **Yield stress** — **R ~ Normal(40000, 2000)**
  - **Young's modulus** — **E ~ Normal(2.9e7, 1.45e6)**
  - **Horizontal load** — **X ~ Normal(500, 100)**
  - **Vertical load** — **Y ~ Normal(1000, 100)**
- **Constants: L = 100in and D_0 = 2.2535 in (max displacement)**

Exploring Parameter-Response Relationship: Vector Parameter Study

- **GOAL: assess global trend of f(x1, x2) along a line in parameter space**

- **Example: 11 equally-spaced samples along a vector in the *x1-x2* parameter space (based on start point, end point, number of samples)**

- **Not especially useful with N=2, but can be when N>2**
  - **With large steps, provides some global trend info on function values**
  - **With small steps, provides some local trend info on f-values (quasi-derivatives)**



See User's Manual Section 2.4.1.2

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Running a Vector Parameter Study

- If using JAGUAR:
  - Start JAGUAR (`Jaguar` command) and set the DAKOTA executable location in Window > Preferences > Jaguar
  - Create a new file from template: "Parameter Study Vector"
- If using a text editor, copy to a location of your choice: `Dakota/examples/tutorial/dakota_rosenbrock_vector.in`
- Discuss the sections of this DAKOTA input file
- Verify the example runs (running in JAGUAR can be slower):
  - Use JAGUAR "Execute Problem" tab: "Check" and "Run"; or
  - Run `dakota -input myvector.in` from the command line (try `-check`)
- Modify this problem for cantilever (2 design, 4 state variables)
- See DAKOTA reference manual locally or at http://dakota.sandia.gov/documentation.html

Input File:
Vector Parameter Study

```
# DAKOTA INPUT FILE - dakota_rosenbrock_vector.in

strategy,
          single_method
            graphics,tabular_graphics_data

method,
          vector_parameter_study
            final_point = 1.1  1.3
            num_steps = 10

model,
          single

variables,
          continuous_design = 2
            initial_point   -0.3      0.2
            descriptors      'x1'     "x2"

interface,
          direct
            analysis_driver = 'rosenbrock'

responses,
          num_objective_functions = 1
          no_gradients
          no_hessians
```

JAGUAR Guides Creation of Dakota Input Deck

6 potential sections (2 optional, 4 required):

Define Problem

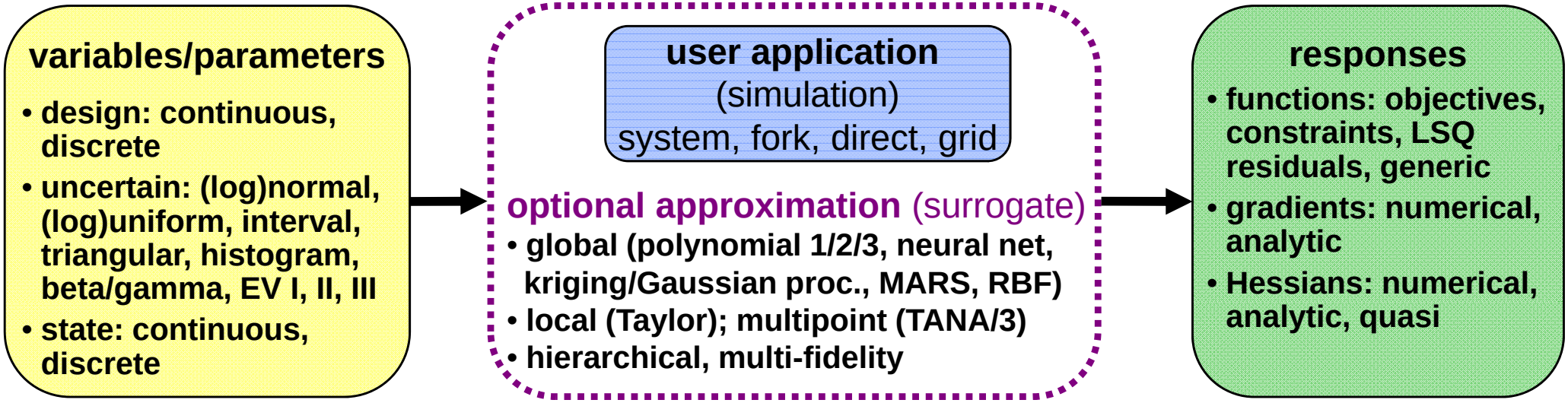
- Model *(optional):* single, surrogate (global, local, hierarchical), nested
- Variables *(required):* design, uncertain, and state variables; continuous/discrete
- Interface *(required):* system call, fork, or direct; specify parallel options
- Responses *(required):* number of responses/constraints, gradients, Hessian

Define Flow

- Strategy *(optional): coordination of methods* single_method, hybrid, multi_start, pareto_set
- Method *(required):* parameter studies, nondeterministic methods, optimization methods

Optional Info: Flexibility with Models

DAKOTA models map inputs to response metrics of interest:



integrate parameters into application inputs

extract relevant metrics

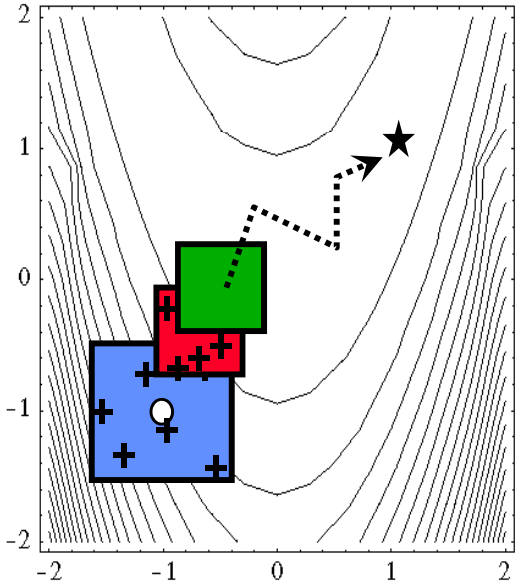
For all DAKOTA studies, must specify the:

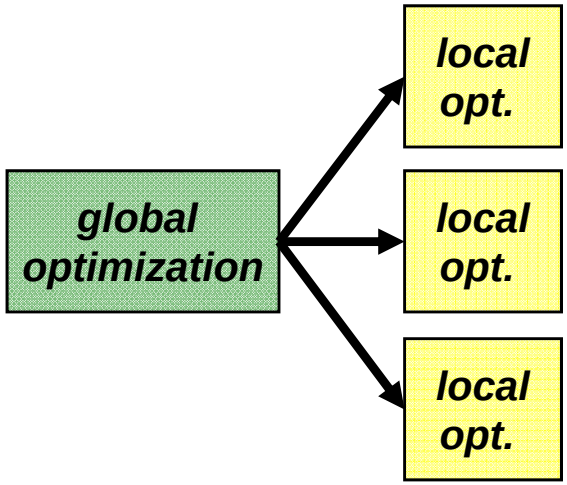
- **variables of interest (types vary by study),**
- **interface that evaluates them**
- **responses it produces**

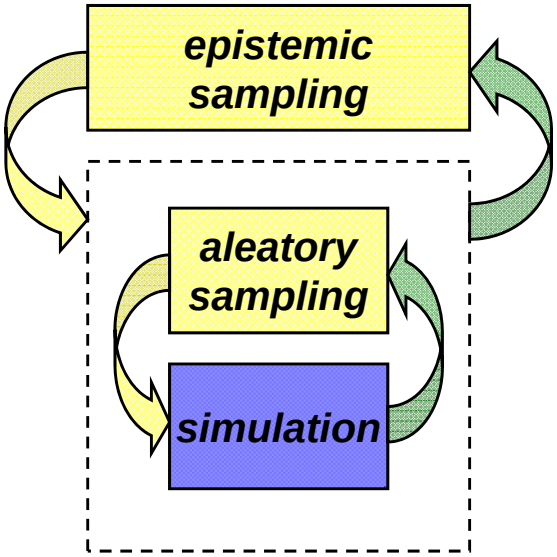
Optional Info: Strategies (and advanced/multi-component methods)

***Strategies** (nesting, layering, sequencing and recasting facilities) combine methods to enable advanced studies:*

- **Combine optimization/calibration with uncertainty quantification**
- ***Surrogate-based approaches***
- ***Hybrid optimization***
- **Nested UQ**







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Explore Cantilever Along a Vector in *w-t* Space

- Start with `dakota_rosenbrock_vector.in` (Parameter Study Vector)
- Modify to explore variables `beam_width` and `beam_thickness` on [1.0, 4.0]
- The `mod_cantilever` driver requires specification of all 6 variables, so add state variables to keep the uncertain variables fixed at means:

```
continuous_state = 4
  initial_state  40000. 29.E+6 500. 1000.
  descriptors      'R'   'E'   'X'   'Y'
```

- Add identical values to `final_point` so *R, E, X* and *Y* don't vary
- Change the analysis_driver to `'mod_cantilever'`
- Cantilever has 3 response functions, instead of 1; specify descriptors `'area' 'stress' 'displacement'`
- See DAKOTA reference manual: method, variables, responses commands (http://dakota.sandia.gov/documentation.html)

Potential Solution: Cantilever Vector Parameter Study

```
# extraexamples/cantilever_vector.in

strategy,
  single_method
  graphics, tabular_graphics_data

method,
  vector_parameter_study
         final_point = 4.0 4.0 40000. 29.E+6 500. 1000.
         num_steps = 10

variables,
  continuous_design = 2
         initial_point   1.0      1.0
         descriptors      'beam_width'     'beam_thickness'
  continuous_state = 4
         initial_state  40000. 29.E+6 500. 1000.
         descriptors      'R'   'E'   'X'   'Y'

interface,
  direct
         analysis_driver = 'mod_cantilever'

responses,
  num_objective_functions = 3
         response_descriptors = 'area' 'stress' 'displacement'
  no_gradients
  no_hessians
```

Dakota Execution and Output

- DAKOTA is most commonly run from a UNIX or Windows command prompt

- Capture output: input variable and response information for each function evaluation; method-specific info

```
>> dakota –i my_run.in –o my_run.out
```

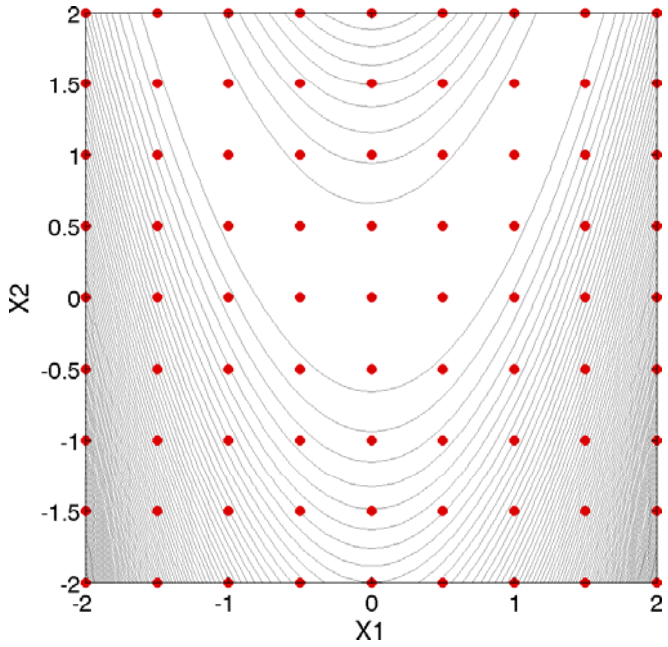
- If strategy includes `tabular_graphics_data`, generates tabular listing of inputs and outputs, called `dakota_tabular.dat`. Useful for Excel, Matlab, or other package import.

- *Other command-line options*

```
>> dakota –help
```

Exercise: Multi-dimensional Parameter Study

- **Goal: understand how responses *area, stress, and displacement* vary with respect to the inputs *w* and *t* on a grid of points.**
- ***Exercise: change previous input file to run the mod_cantilever computational model at a grid of points over [1.0, 4.0] using the*** `multidim_parameter_study` ***method***
- **Try 9 points in one dimension, 6 in the other**
- **See method and variable commands in DAKOTA reference manual**
- **What parts of the file did you have to change?**



Example: uniform grid over [-2.0, 2.0]

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Sample Input File: Multi-dimensional Parameter Study

```
# extraexamples/cantilever_grid.in
strategy,
single_method
  graphics,tabular_graphics_data

method,
multidim_parameter_study
  partitions = 9 6 0 0 0 0

variables,
continuous_design = 2
  lower_bounds   1.0      1.0
  upper_bounds   4.0      4.0
  descriptors      'beam_width'     'beam_thickness'
continuous_state = 4
  lower_bounds  40000. 29.E+6 500. 1000.
  upper_bounds  40000. 29.E+6 500. 1000.
  descriptors      'R'   'E'   'X'   'Y'

interface,
direct
  analysis_driver = 'mod_cantilever'

responses,
num_objective_functions = 3
    response_descriptors = 'area' 'stress' 'displacement'
no_gradients
no_hessians
```

DAKOTA 101: Coming Up

Method Tour

- Sensitivity Analysis
- Uncertainty Quantification
- Optimization and Calibration
- Advanced Topics per class interest and time

Additional Topics
(revisit later today per 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)