SAND2011-1868C

DAKOTA Overview and Application Examples

ORNL/RNSD/SCALE
March 8, 2011

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Optimization and Uncertainty Quantification (01441)

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DAKOTA Overview Goals

GOAL: Help you decide if DAKOTA might be relevant for your work

- Overview of DAKOTA, key capabilities
- Four categories of methods, with examples
- Getting Started
- *Choose your adventure:*
  - Advanced capabilities (models, strategies, parallelism)
  - JAGUAR graphical user interface
  - Interfacing with DAKOTA (script and library)

DAKOTA plays a key role in

- risk-informed analysis and design of engineered systems (with structural, thermal, electrical, and other phenomena),
- nuclear energy initiatives (including CASL, NEAMS), as well as
- product R&D and scientific discovery worldwide.

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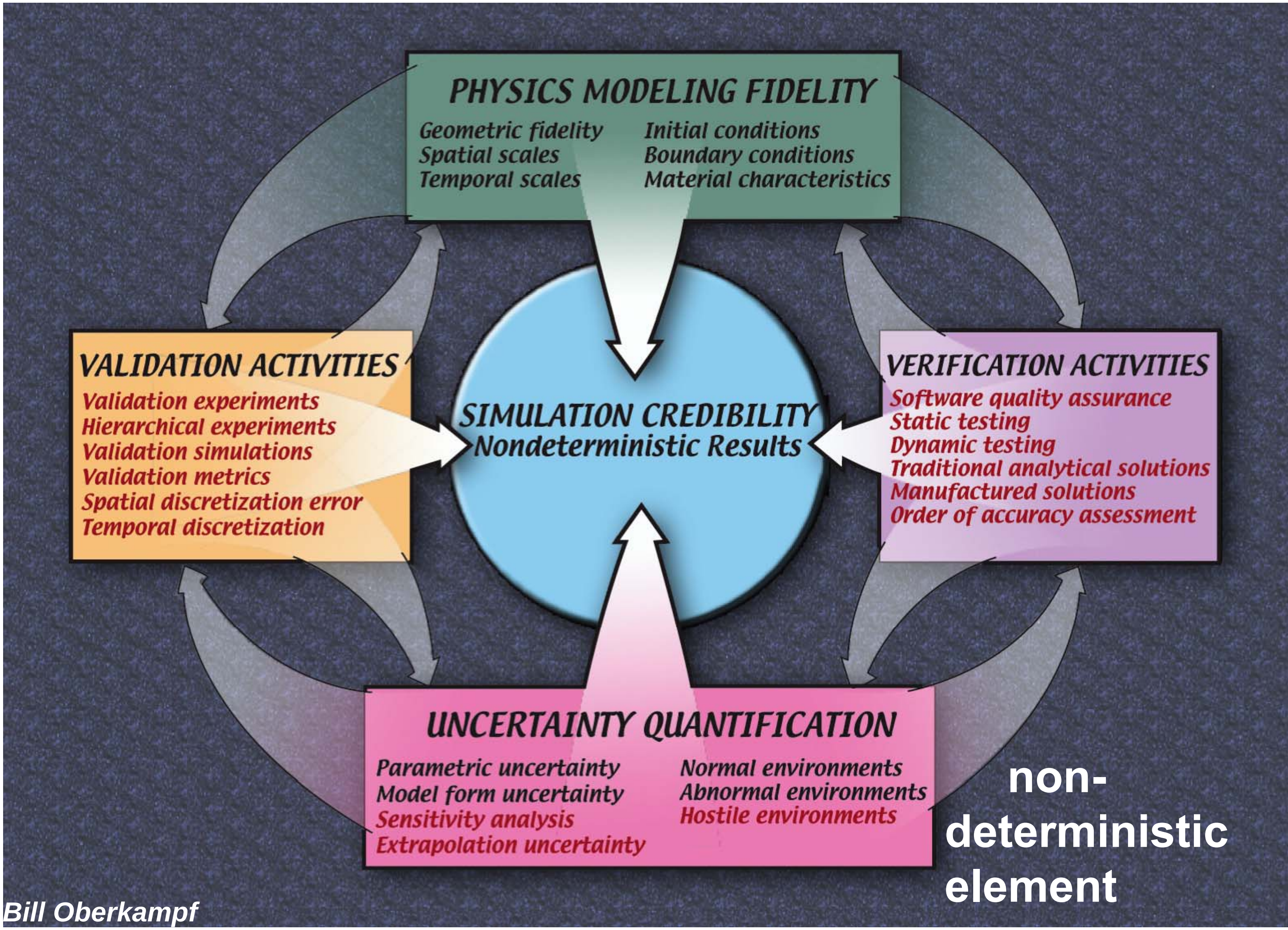
V&V, UQ, and Model Fidelity Support Credible Simulation

Insight, prediction, and risk-informed decision-making
require credibility for intended application



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***

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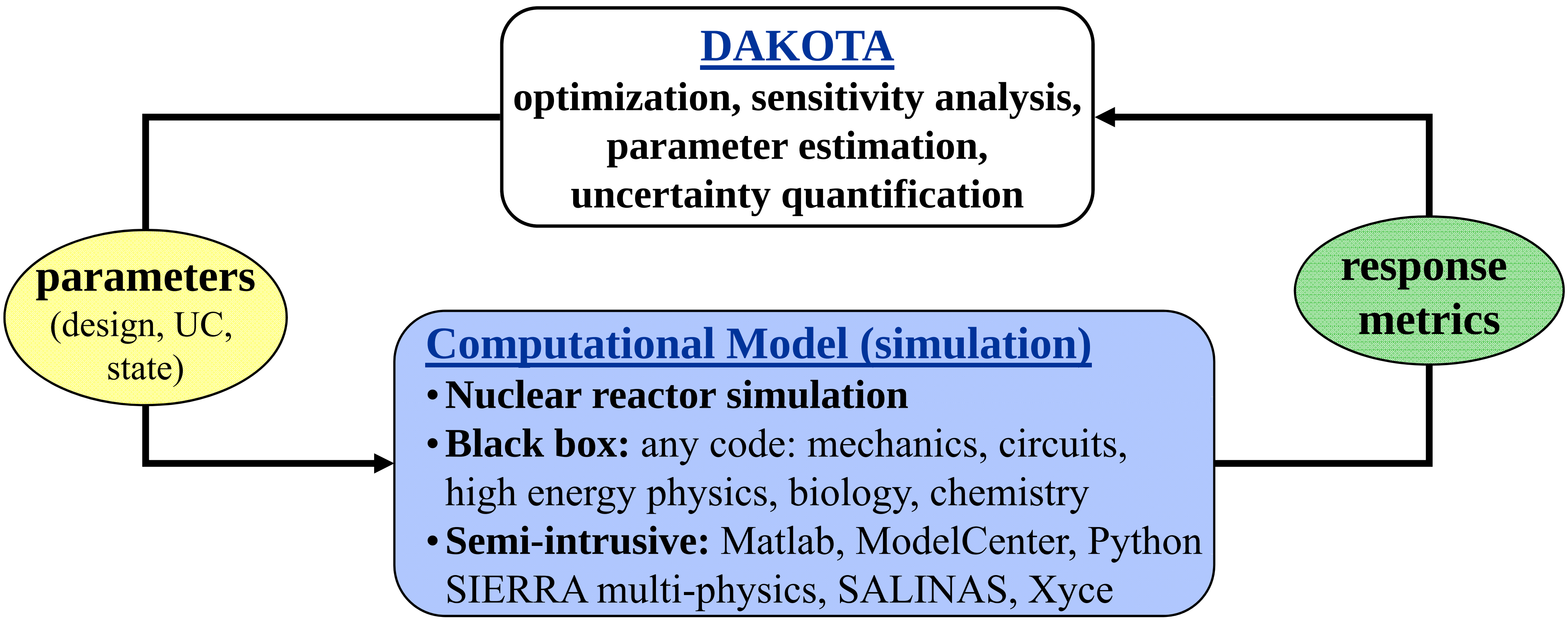
Automated Iterative Analysis

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



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

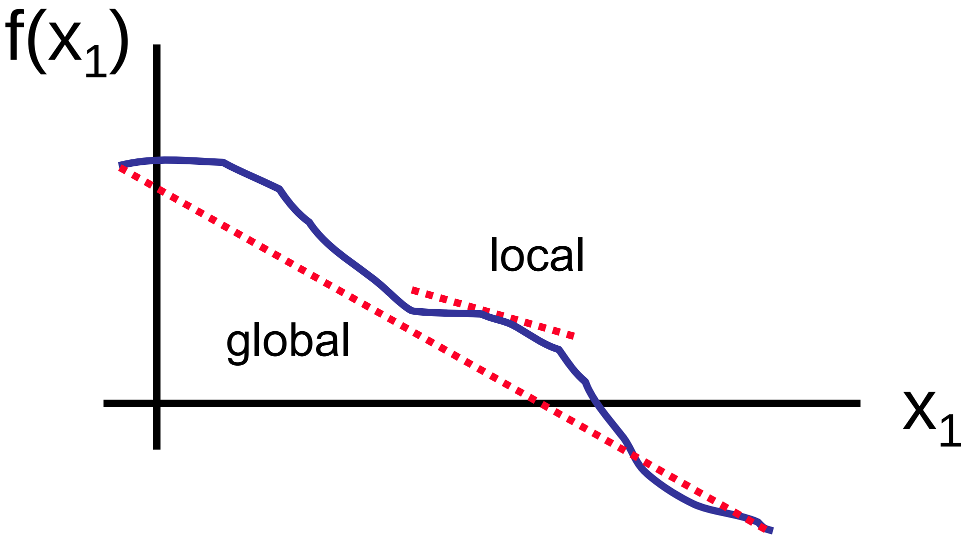
Key DAKOTA Capabilities

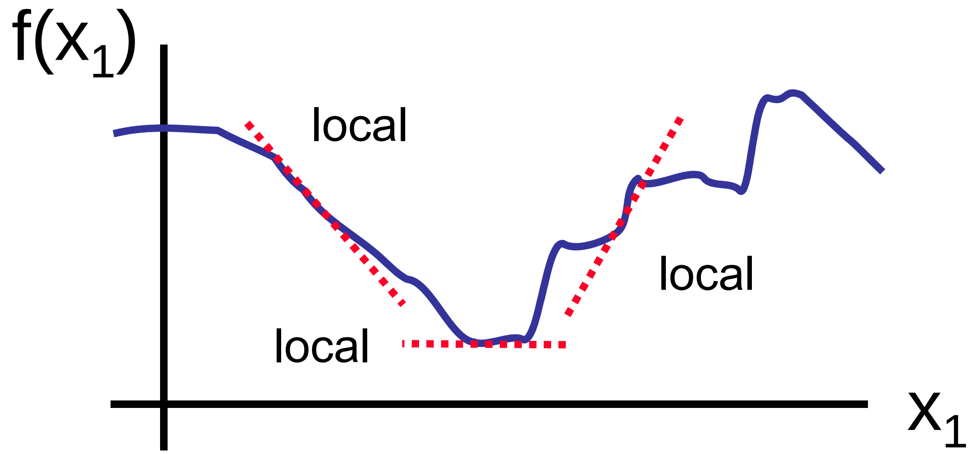
- Generic interface to simulations
- Time-tested and advanced algorithms to address nonsmooth, discontinuous, multimodal, expensive, mixed variable, failure-prone
- Strategies to combine methods for advanced studies or improve efficiency with surrogates (meta-models)
- Mixed deterministic / probabilistic 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 mailing lists
  - Software downloads: stable releases and nightly builds (freely available worldwide via GNU LGPL)

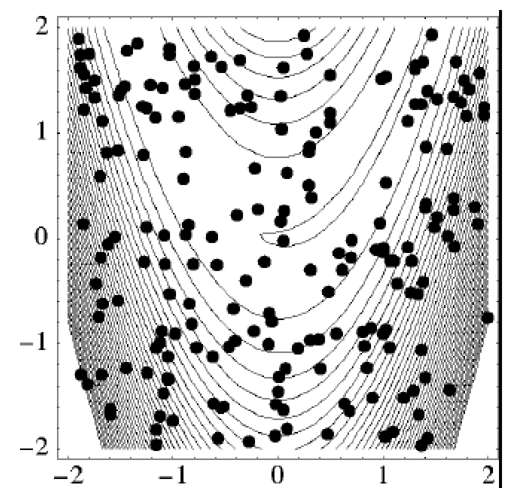
Sensitivity Analysis

How do code outputs vary due to changes in code inputs?





- **Sensitivity analysis examines variations in $f(x_1)$ due to perturbations in x_1**
  - **Local sensitivities are typically partial derivatives (given a specific x1, what is the slope at that point?)**
  - **Global sensitivities are typically found via sampling methods and regression (what is the trend of the function over all values of x1?)**
- **Determines which variables are important to perform optimization or UQ on, or which to gather more data on or control in an experiment.**



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SA Examples for Nuclear Energy

- Which thermal hydraulic parameters (temperature, pressure, flow rate, power input, etc.) most influence localized boiling and consequently, formation of boron deposits (and CRUD in general) and related power reduction. In what way?

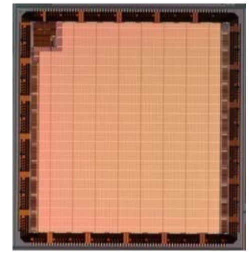
- Which structural or fluid characteristics most affect the seriousness of grid-to-rod fretting?

- How do cross section data uncertainties influence criticality of new sodium fast reactor designs?

- Which system safety components most likely lead to serious accident scenarios?

SA for Electrical Circuits

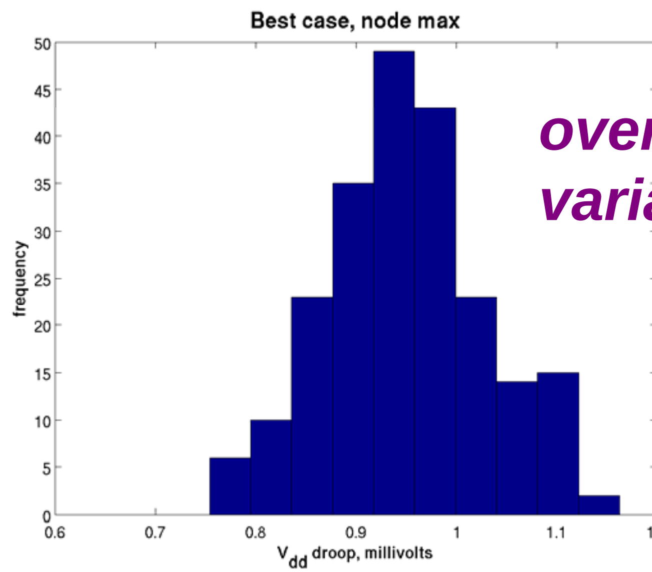
- **CMOS7 ViArray:** generic ASIC implementation platform; *applications in NW, satellite, command & control*
- Modeling and simulation used in design phase to assess predicted performance during photocurrent event, including sensitivity/variability of supply voltage
- DAKOTA coupled to Xyce circuit simulator to **determine which process layers contributed most to device performance** (1000s of simulation runs, each 2.0h to 4.5h)



Xyce™ Parallel Electronic Simulator

	Vdd Metrics	
	node max	node avg
METAL1	0.96	0.82
METAL2	0.11	0.04
METAL3	0.10	0.05
METAL4	0.80	0.81
METAL5	0.86	0.91
VIA1	0.71	0.66
VIA2	0.80	0.76
VIA3	0.57	0.60
VIA4	0.91	0.94
CONTACT	0.21	0.13
polyc	0.04	0.05

correlations



overall variability

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DAKOTA Sensitivity Analysis

- Parameter study, design and analysis of computer experiments, and general sampling methods (heavy global focus):
  - Single and multi-parameter studies (grid, vector, centered)
  - DDACE (grid, sampling, orthogonal arrays, Box-Behnken, CCD)
  - FSUDACE (Quasi-MC, CVT)
  - PSUADE (Morris designs)
  - Monte Carlo, Latin hypercube sampling (with correlation or variance analysis, including variance-based decomposition)
  - Mean-value with importance factors
  - Stochastic expansion (PCE/SC) yielding Sobol indices

- DAKOTA outputs can include correlations, main/total effects, interaction effects; tabular output can be analyzed with any third-party statistics package
- Determine main effects and key parameter *interactions*
- In SA, typically no distribution assumption

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Uncertainty Quantification

Forward propagation: quantify the effect that uncertain (nondeterministic) input variables have on model output

<u>Input Variables *u*</u>
(physics parameters, geometry, initial and boundary conditions)

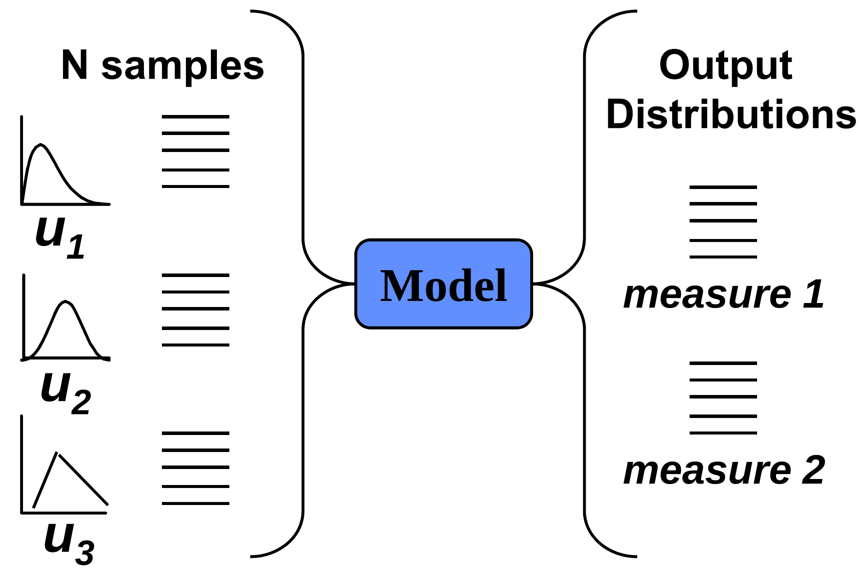
→ **Computational Model** →

Variable Performance Measures *f(u)*

(possibly given distributions)

Potential Goals:

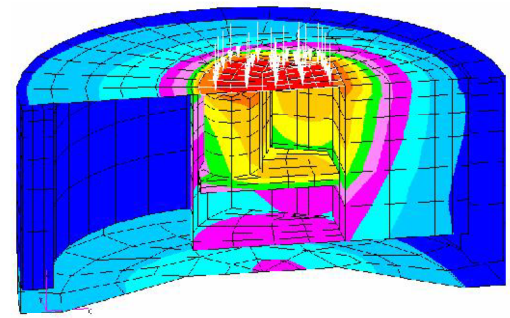
- **based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)**
- **validation: is the model sufficient *for the intended application?***
- **quantification of margins and uncertainties (QMU): *how close are uncertainty-aware code predictions to performance expectations or limits?***
- ***quantify uncertainty when using calibrated model to predict***

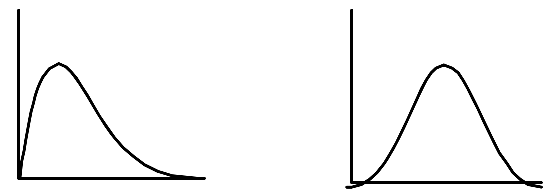


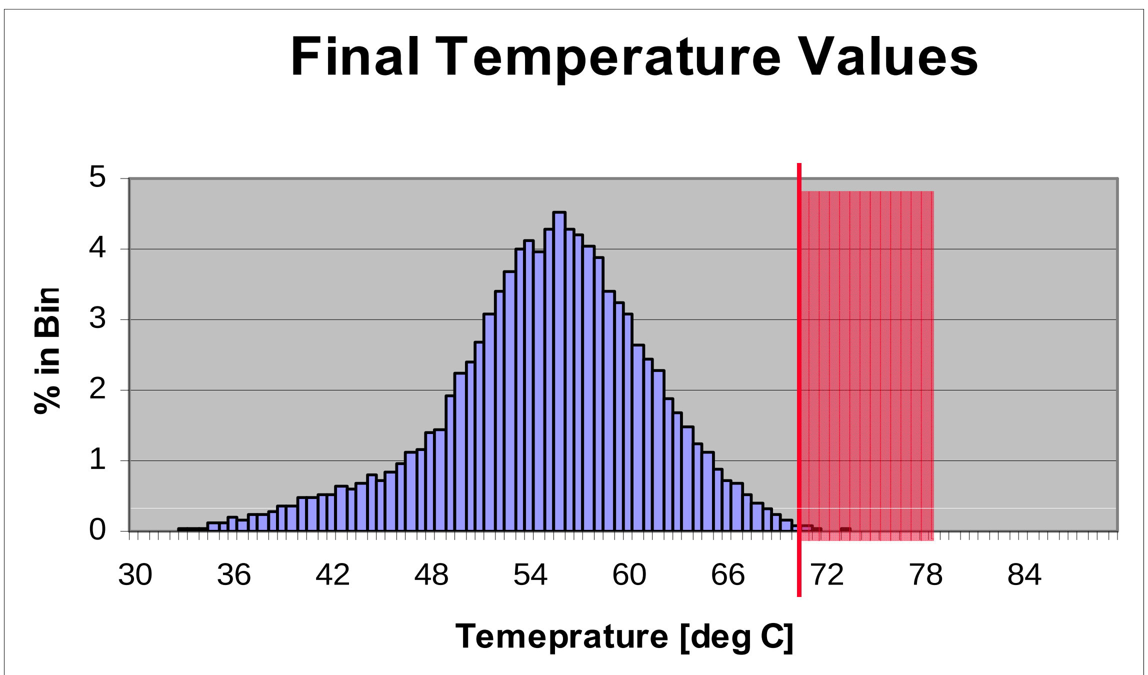
Typical method: Monte Carlo Sampling

Thermal
Uncertainty Quantification

- **Device subject to heating** **(experiment or computational simulation)**
- **Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by** $u_1, \ldots, u_N$
- **Response temperature** $f(u)=T(u_1, \ldots, u_N)$ **calculated by heat transfer code**







Given distributions of $u_1,\ldots,u_N$***, UQ methods calculate statistical info on outputs:***

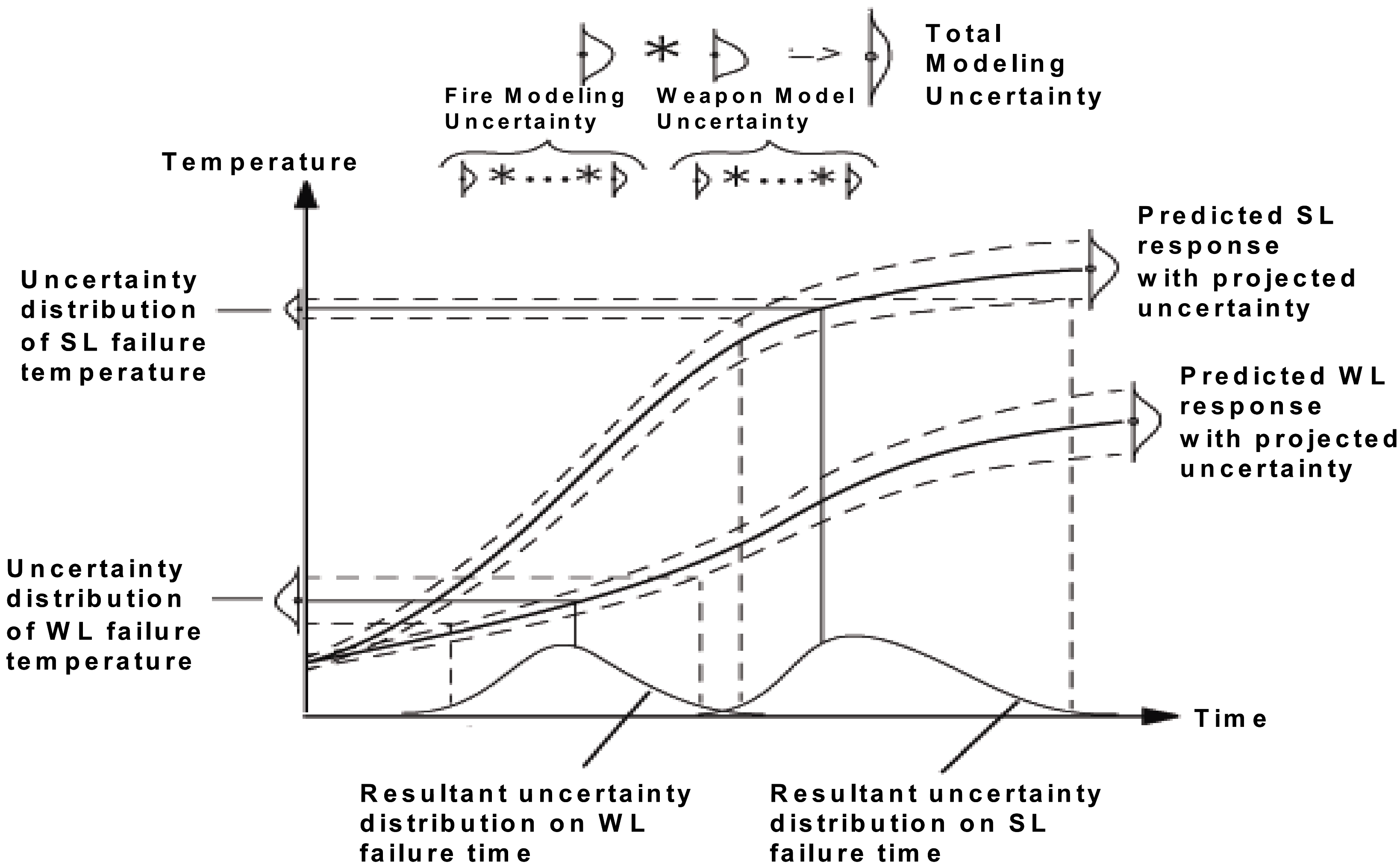
- **Mean(*T*), StdDev(*T*), Probability(**$T \geq T_{critical}$**)**
- **Probability distribution of temperatures**
- ***Correlations (trends) and sensitivity of temperature***

UQ Examples for Nuclear Energy

- **What are mean, standard deviation, and distribution of a response (peak coolant temperature), given distributions on input parameters: pump power lost, SCRAM delay, control rod injection distance, etc.?**

- **Given uncertainties in fuel composition, flow rates, and formation of by-products, what is the probability of excessive localized boiling under a particular operating condition?**

UQ for Thermal Race



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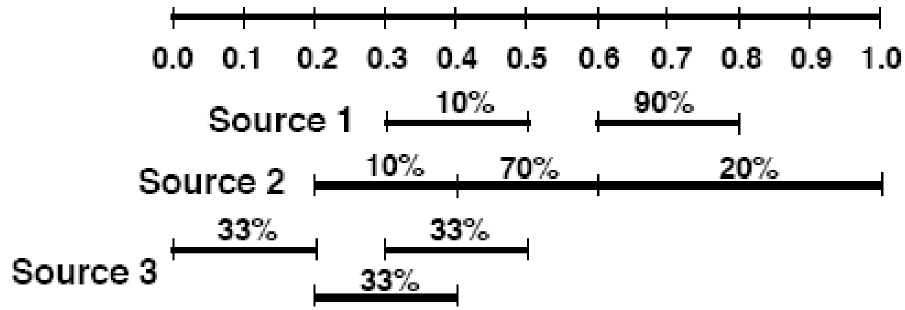
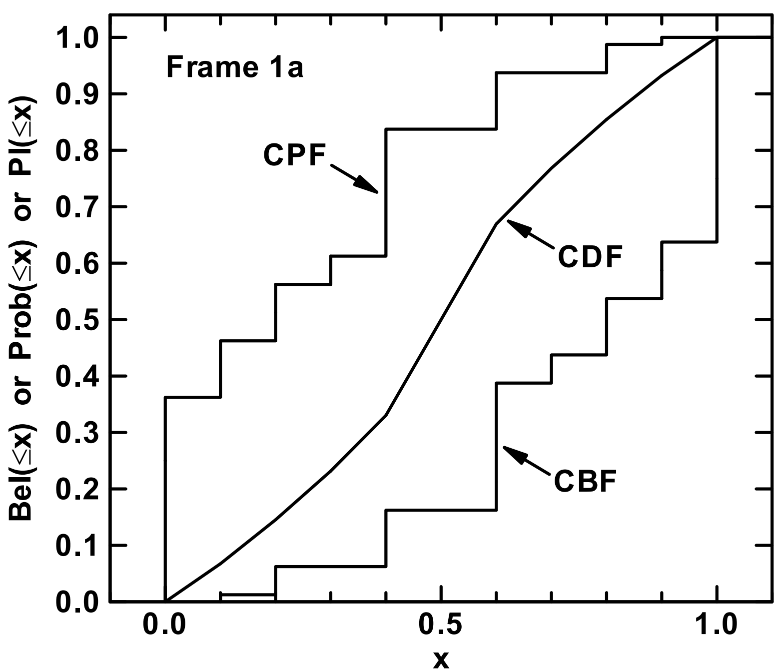
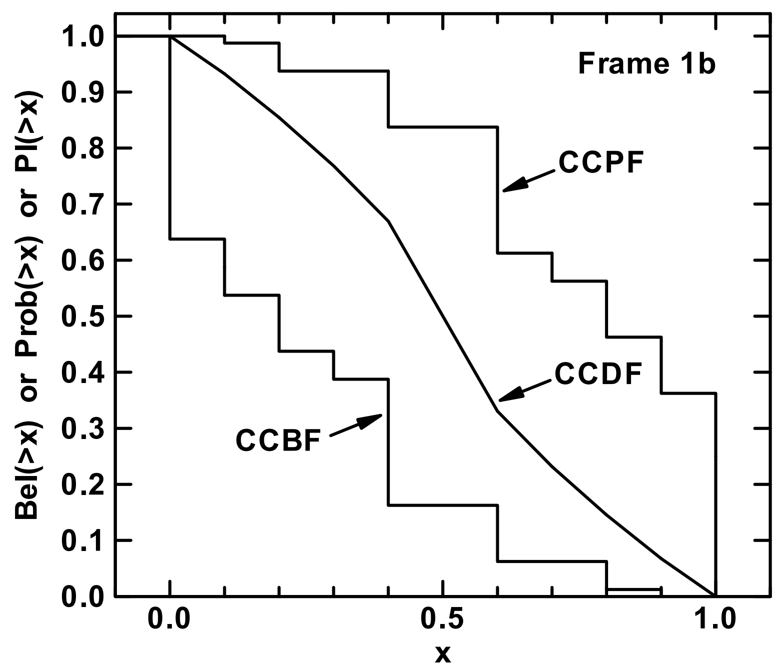
Dempster-Shafer Theory

Intervals on the inputs are propagated to calculate



- **Belief:** a lower bound on a probability value that is consistent with the evidence
- **Plausibility:** an upper bound on a probability value that is consistent with the evidence.





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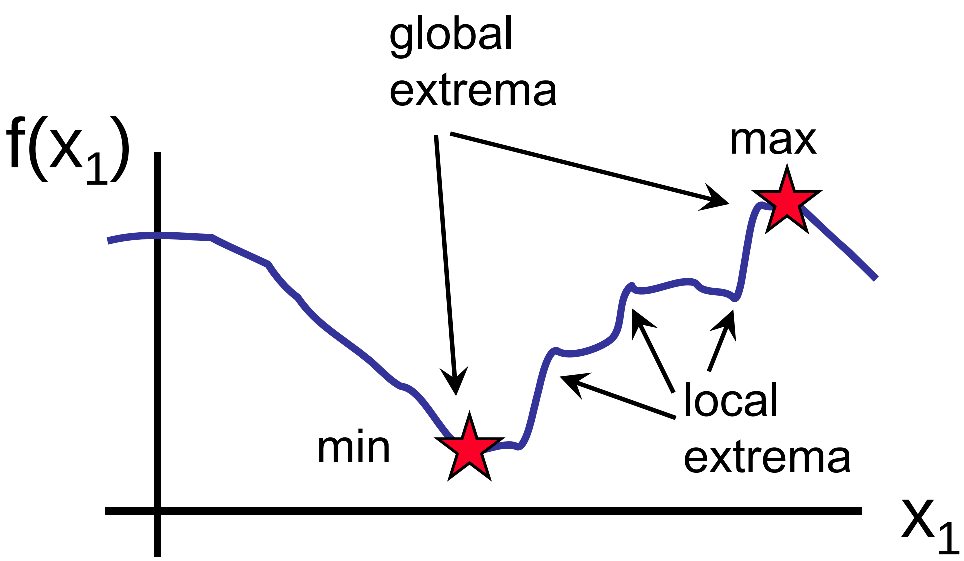
DAKOTA UQ

- Techniques for propagating aleatory uncertainty (variables characterized by probability distributions) through models:
  - Latin hypercube (and other) sampling
  - Local reliability methods (mean value, MPP search, FORM, SORM)
  - Global reliability methods (EGRA)
  - Non-intrusive stochastic expansion methods (polynomial chaos and stochastic collocation)
  - *Reliability and importance sampling help with low probability events*
- Methods for epistemic uncertainty (variables characterized by intervals or basic probability assignments):
  - Local/global interval estimation
  - Local/global Dempster-Shafer evidence theory (belief/plausibility)
  - “Second-order” probability via sampling

- DAKOTA can output moments, probability of response thresholds, reliability metrics, response corresponding to a metric, etc.

Optimization

- **GOAL: Vary parameters to extremize objectives, while satisfying constraints to find (or tune) the best design, estimate best parameters, analyze worst-case surety, e.g., determine:**
  - **delivery network that maximizes profit while minimizing environmental impact**
  - **case geometry that minimizes drag and weight, yet is sufficiently strong and safe**
  - **material atomic configuration of minimum energy**



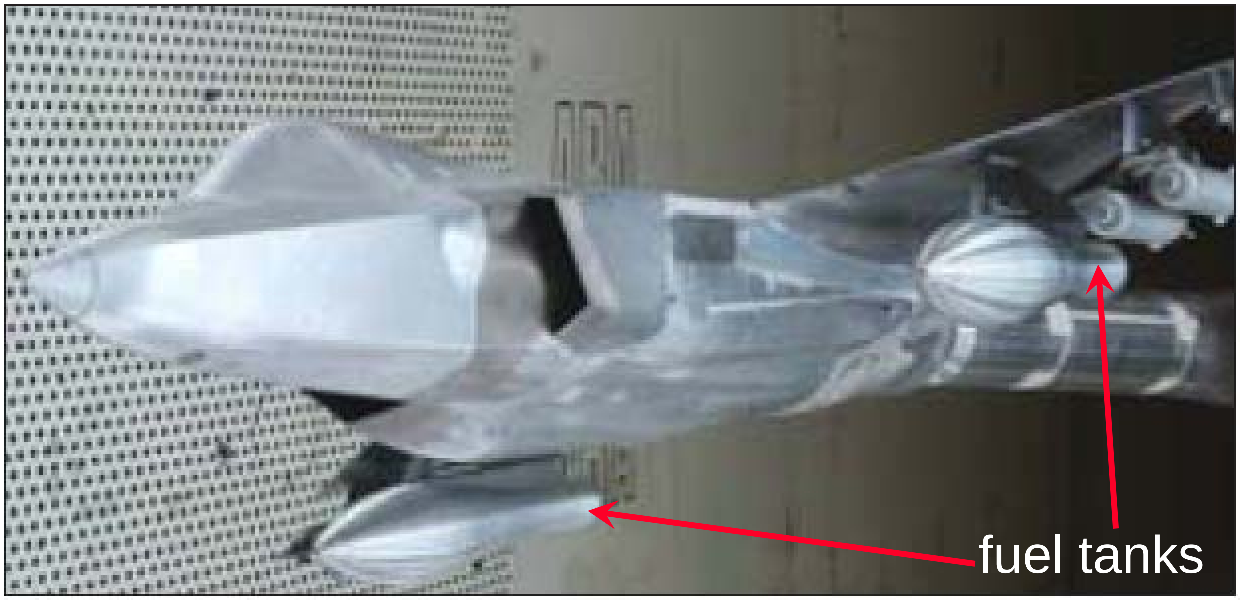
Some applications: local improvement suffices; others: must find global minimum at any cost

Optimization Examples for Nuclear Energy

- What fuel re-loading pattern yields the smoothest reactor power distribution while maximizing output?

- Can we adjust flow rates, pressures, etc., to reduce likelihood of CRUD-induced power shift (CIPS)?

Optimization for Lockheed-Martin F-35 External Fuel Tank Design



This wind tunnel model of F-35 features an optimized external fuel tank.

F-35: stealth and supersonic cruise

~ $20 billion cost

~ 2600 aircraft (USN, USAF, USMC, UK & other foreign buyers)

LM CFD code:

- ***Expensive*: 8 hrs/job on 16 processors**
- **Fluid flow around tank *highly sensitive* to shape changes**

"Lockheed Martin Aeronautics conducted a trade study for the F-35 Joint Strike Fighter (JSF) aircraft to design the external fuel tank for improved performance, store separation, and flutter. **CFD was used in conjunction with Sandia National Laboratories' Dakota optimization code to determine the optimal shape of the tank that minimizes drag for maximum range and minimizes yawing moment for separation of adjacent stores.** Data obtained at several wind tunnel facilities verified the predicted performance of the new aeroshaped, compartmented tank for separation and flutter, as well as acceptable characteristics for loads, stability, and control." -- Dec. 2004 *Aerospace America*, p. 22

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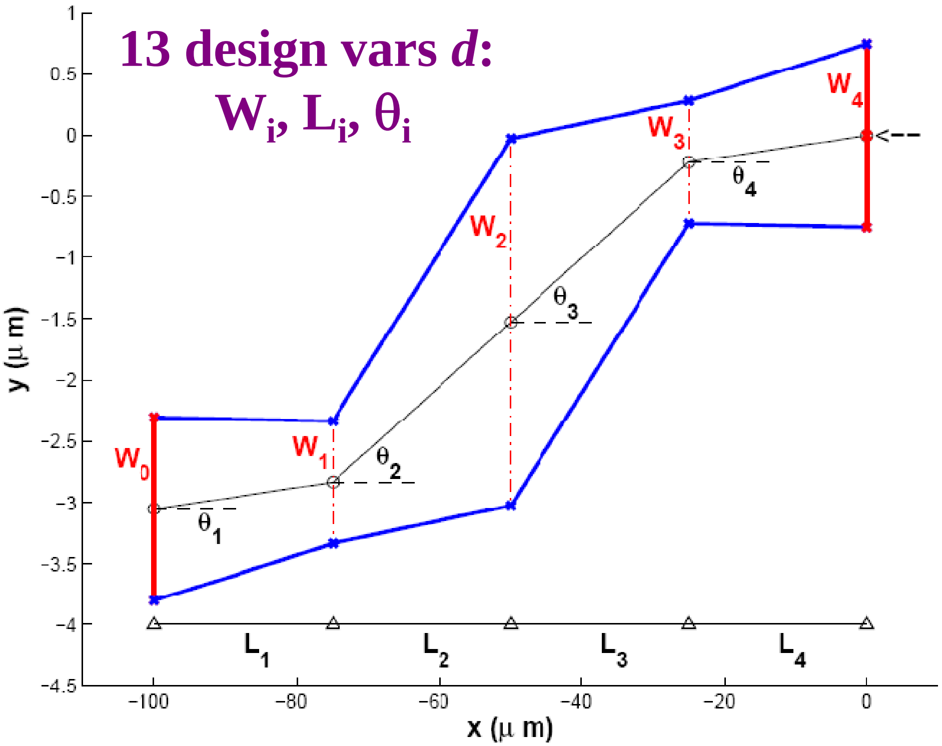
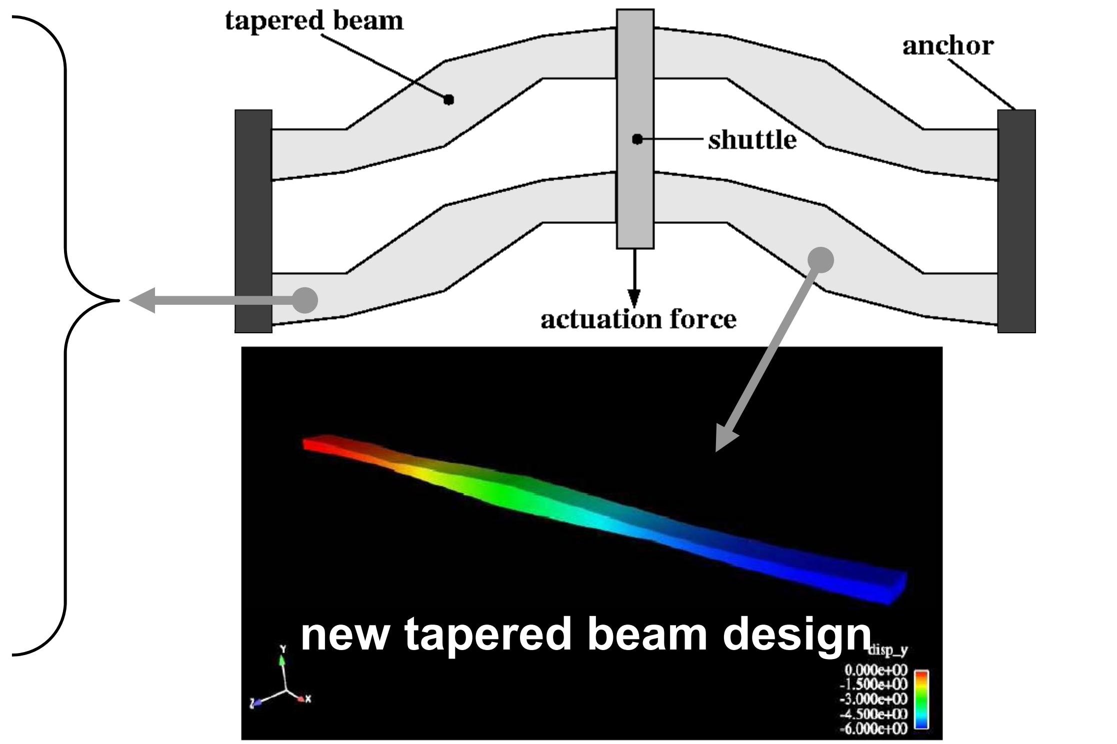
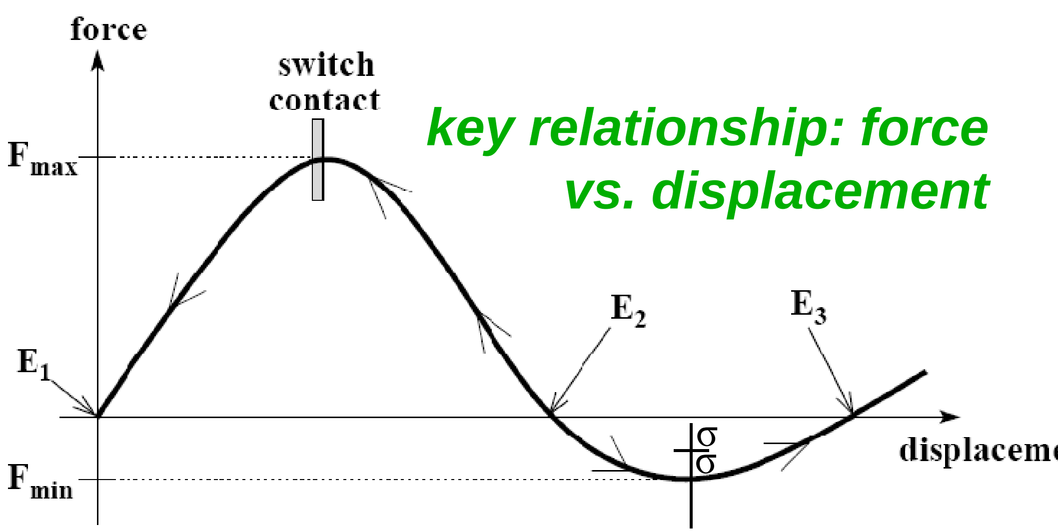
MEMS Switch Design: Geometry Optimization







key relationship: force vs. displacement

Typical design specifications:

- actuation force F_{min} reliably 5 μN
- bistable ($F_{max} > 0$, $F_{min} < 0$)
- maximum force: $50 < F_{max} < 150$
- equilibrium E2 < 8 μm
- maximum stress < 1200 MPa

DAKOTA Optimization Methods

Gradient-based methods

(DAKOTA will compute finite difference gradients and FD/quasi-Hessians if necessary)

- ***DOT (various constrained)***
- **CONMIN (FRCG, MFD)**
- ***NPSOL (SQP)***
- ***NLPQL (SQP)***
- **OPT++ (CG, Newton)**

Calibration (least-squares)

- **NL2SOL (GN + QH)**
- ***NLSSOL (SQP)***
- **OPT++ (Gauss-Newton)**

Derivative-free methods

- **COLINY (PS, APPS, Solis-Wets, COBYLA2, EAs, DIRECT)**
- **JEGA (single/multi-obj GAs)**
- **EGO (efficient global opt via Gaussian Process models)**
- **DIRECT (Gablonsky)**
- **OPT++ (parallel direct search)**

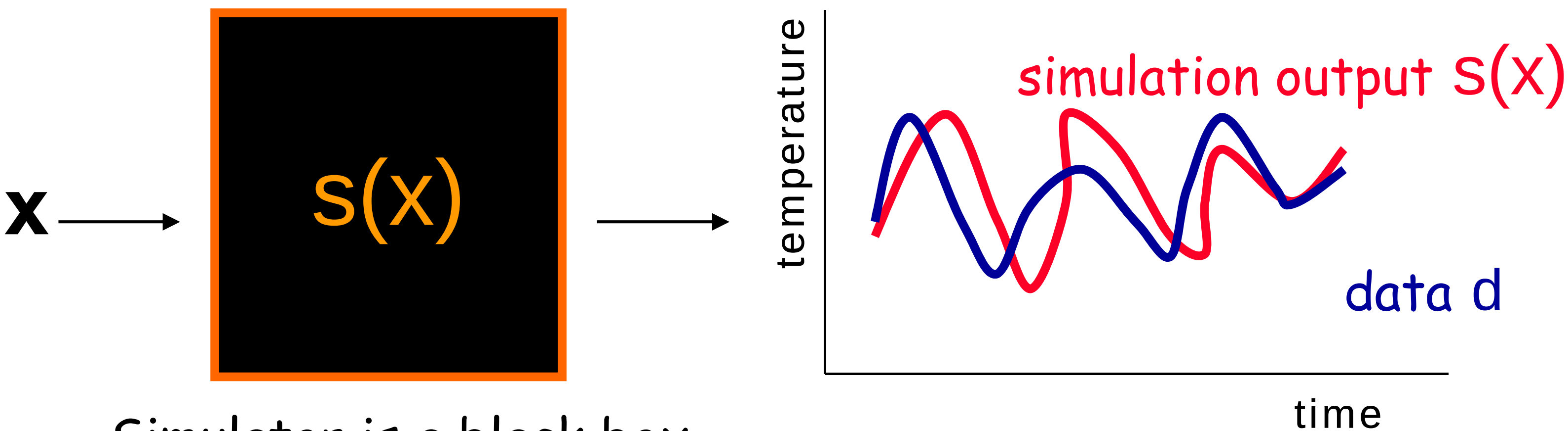
- ***TMF (templated meta-heuristics framework)***

Calibration/Parameter Estimation

$$f(x) = \sum_{i=1}^{n} (s_i(x) - d_i)^2$$

Simulation output that depends on x

Given data



Simulator is a black box

Calibration: Adjust model parameters (x) to maximize agreement with a set of experimental data (AKA parameter estimation, parameter identification, systems, identification, nonlinear least-squares)

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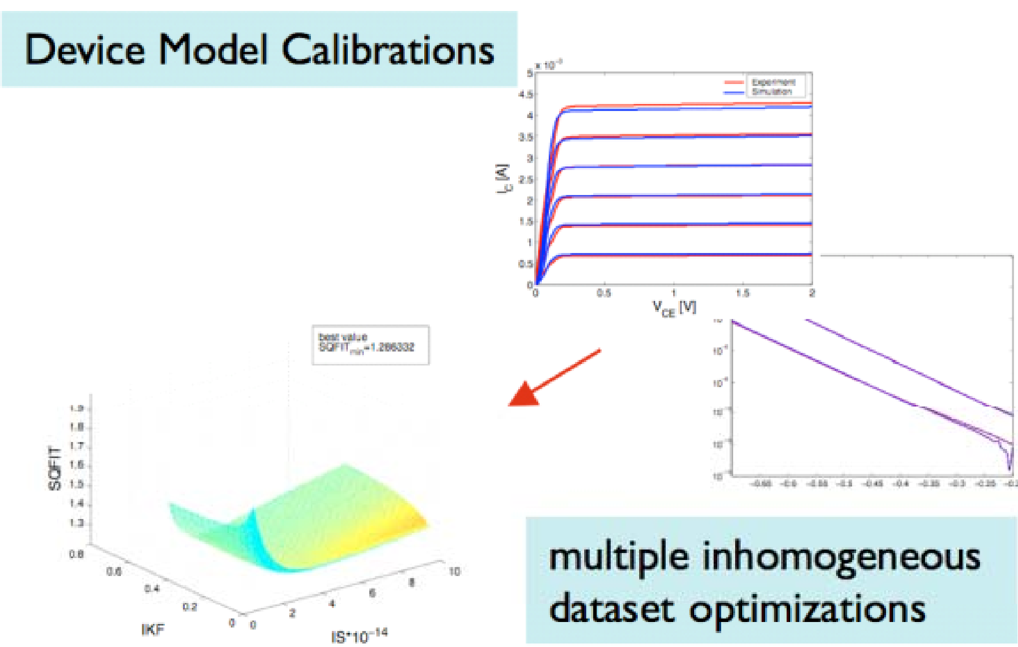
Calibration for Nuclear Energy

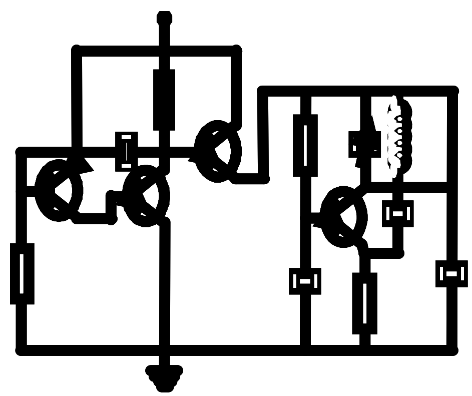
- Data assimilation: use collected operational data to update models of reactor performance and risk.

- Determine which values of neutronics or thermal hydraulic parameters give rise to observed power distributions.

QASPR Model Calibration

- **QASPR Model Calibration:** develop defensible predictive models to replace physical testing with fast neutrons
- Use experimental data to calibrate Complex Prototype Model in Xyce, understand limitations and effects of uncertainty
- HPC runs for parameter screening, determining nominal parameters via calibration, assessing robustness of optima





Getting Started with DAKOTA

- Access a supported installation (preferred) or download the software from DAKOTA webpage
- Attend a DAKOTA training class
- User's Manual, Chapter 2: Tutorial, corresponding examples distributed with DAKOTA
- Support:
  - User forum: `dakota-users@software.sandia.gov` (DAKOTA team and internal/external user community)
  - All support options: `http://dakota.sandia.gov/resources.html`

`http://dakota.sandia.gov/`

DAKOTA Training Classes

New modular format:

- **DAKOTA 101 (intro to using DAKOTA)**
  half day, interactive lecture, optional hands-on (laptop)
- **Interface DAKOTA to your application**
  half day, hands-on small group workshop
- **Advanced topics in DAKOTA User's Group Meetings**
- **Method theory and selection (2 hours each):**
  - **Sensitivity analysis / screening**
  - **Optimization and calibration**
  - **Uncertainty quantification**

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- **product R&D and scientific discovery worldwide.**

Flexibility with Models

DAKOTA models map inputs to response metrics of interest:

variables/parameters
- design: continuous, discrete
- uncertain: (log)normal, (log)uniform, interval, triangular, histogram, beta/gamma, EV I, II, III
- state: continuous, discrete

user application
(simulation)
system, fork, direct, grid

optional approximation (surrogate)
- global (polynomial 1/2/3, neural net, kriging/Gaussian proc., MARS, RBF)
- local (Taylor); multipoint (TANA/3)
- hierarchical, multi-fidelity

responses
- functions: objectives, constraints, LSQ residuals, generic
- gradients: numerical, analytic
- Hessians: numerical, analytic, quasi

integrate parameters into application inputs

extract relevant metrics

Flexible interface to user application (computational model/simulation)

- May be cheap (analytic function, linear analysis); typically costly (finite element mesh with millions of DOF, transient analysis of integrated circuit with millions of transistors)
- Built-in response surfaces/meta-models/surrogates improve efficiency
- May run tightly-coupled, locally as separate process, in parallel on a cluster, remotely on a distributed resource

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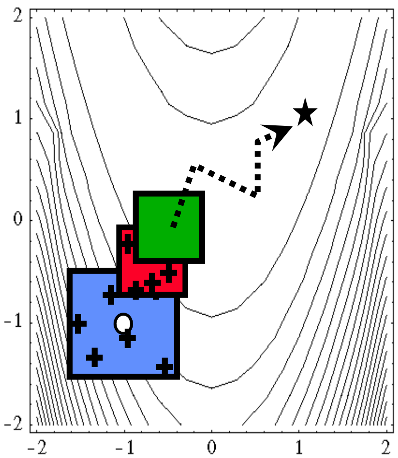
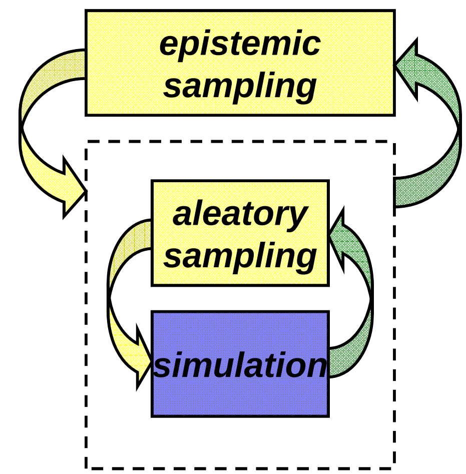
Strategies
(and advanced/multi-component methods)



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

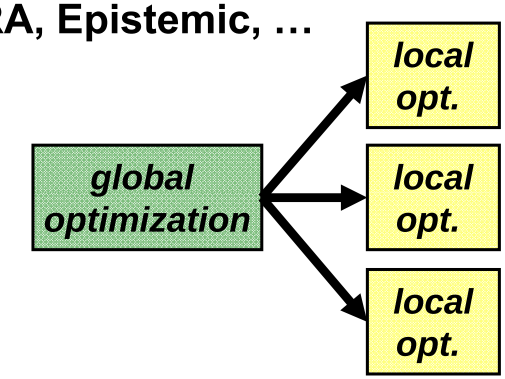
- **opt within opt (multilevel opt & hierarchical MDO)**
- **UQ within UQ (second-order probability)**
- **UQ within opt (OUU) and NLS (MCUU)**
- **opt within UQ (uncertainty of optima)**

with and without surrogate model indirection



Optimization

- **Surrogate-based: data fit, multifidelity, ROM**
- **Mixed integer nonlinear programming (MINLP): PEBBL (parallel branch and bound)**
- **Optimization under uncertainty**
  - **TR-SBOUU, RBDO (Bi-level, Sequential)**
  - **MCUU, PC-BDO, EGO/EGRA, Epistemic, …**
- **Hybrids (e.g., global/local)**
- **Pareto set**
- **Multi-start**
- **Multilevel methods**



Uncertainty

- **Second order probability**
- **Uncertainty of optima**

Nonlinear least squares

- **Surrogate-based calibration**
- **Model calibration under uncertainty**

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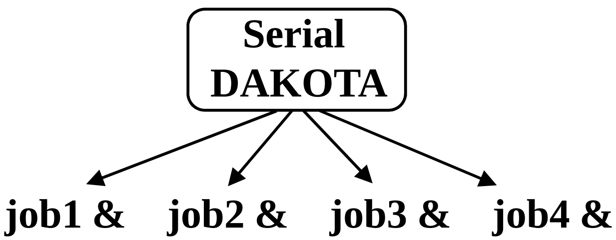
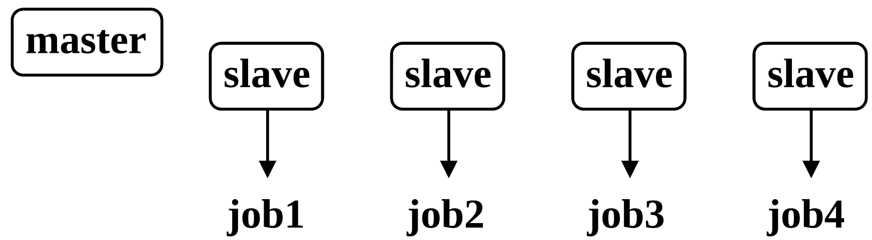
Scalable Parallelism

Nested parallel models support large-scale applications and architectures.

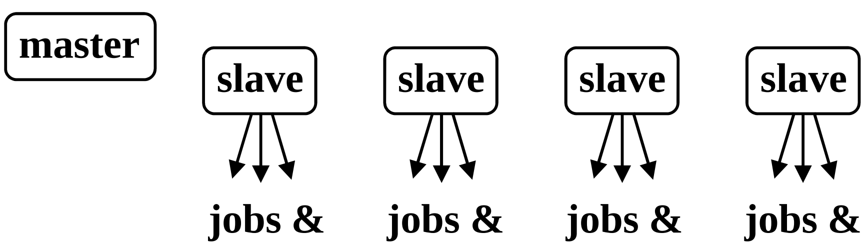
1. SMP/multiprocessor workstations: Asynchronous (external job allocation)



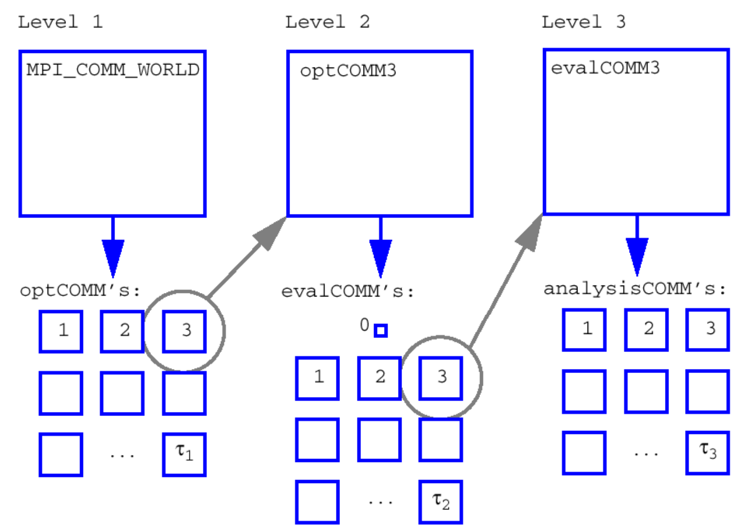
2. Cluster of workstations: Message-passing (internal job allocation)



3. Cluster of SMP's: Hybrid (service/compute model)



4. MPP (Red Storm/ White): Internal MPI partitions (nested parallelism)



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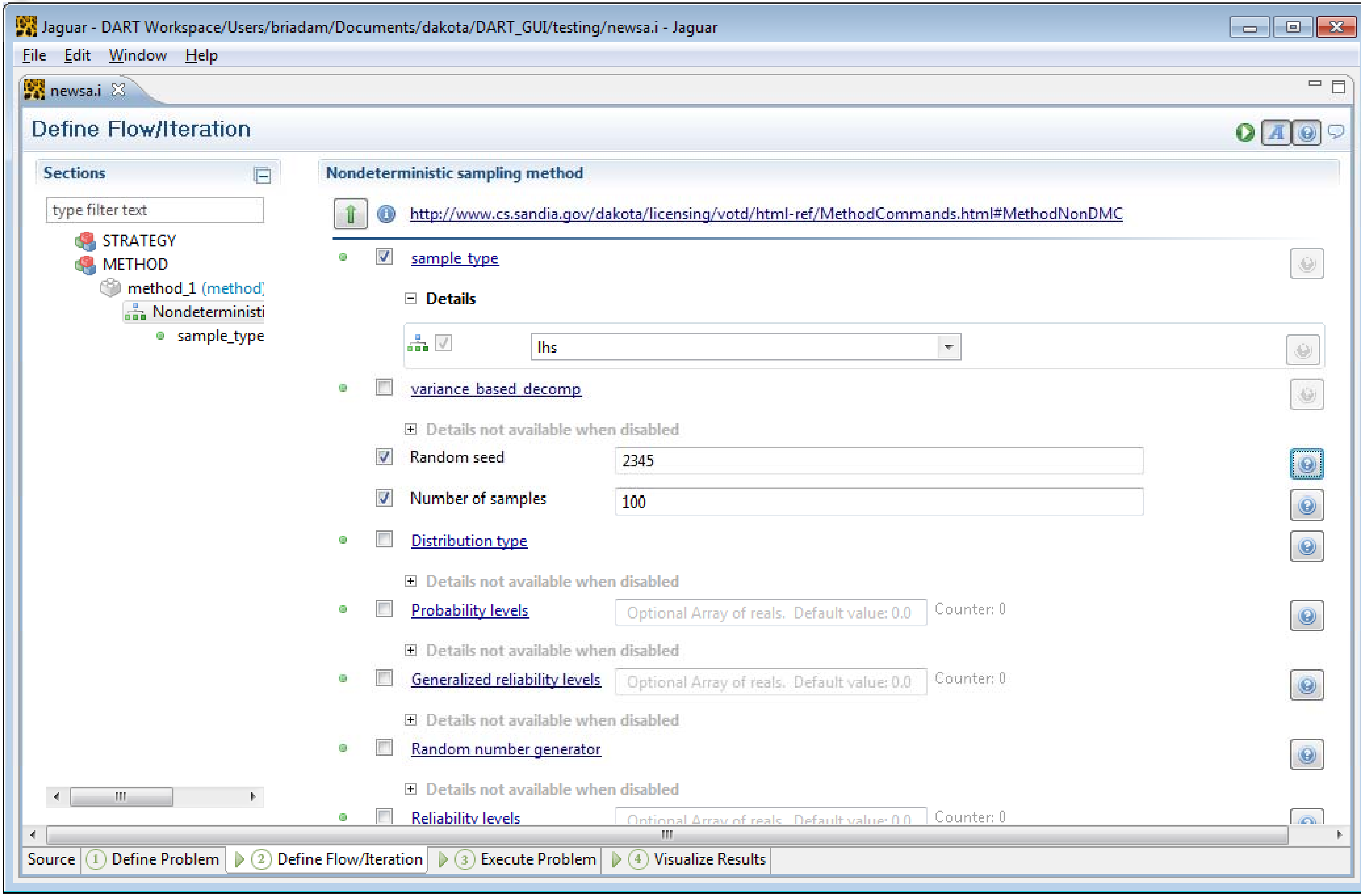
JAGUAR 2.1

- All new graphical user interface for creating, editing, and running DAKOTA input files
- Lead: Ethan Chan (8964), supported by DART and DAKOTA teams

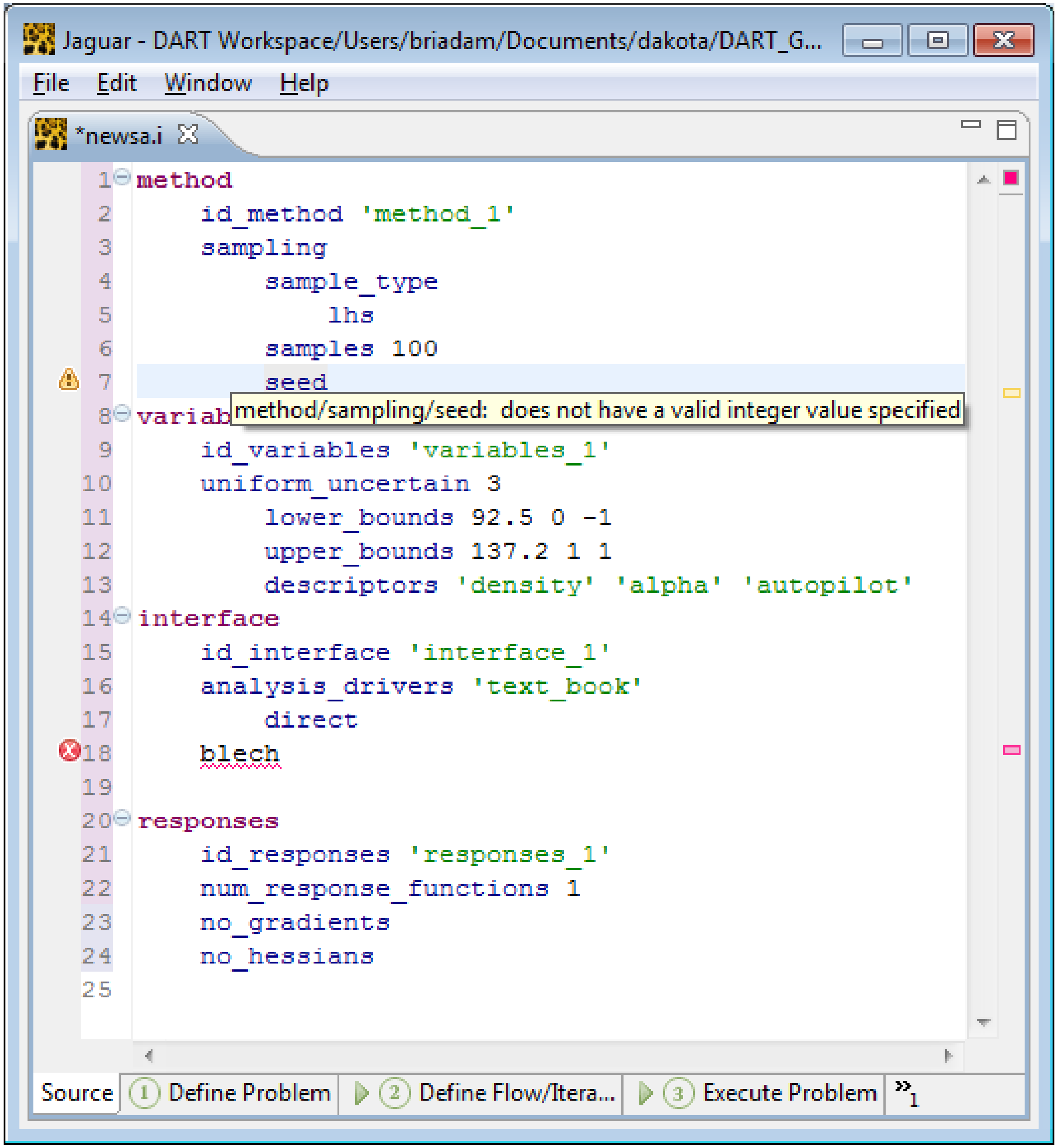
- Java; based on Eclipse IDE/Workbench
- Windows, Mac, Linux support

- Synchronized text and hierarchical graphical editors
- Templates for common studies
- Error checking and integrated help
- Sensitivity analysis wizard

JAGUAR Graphical Editor



JAGUAR Text Editor



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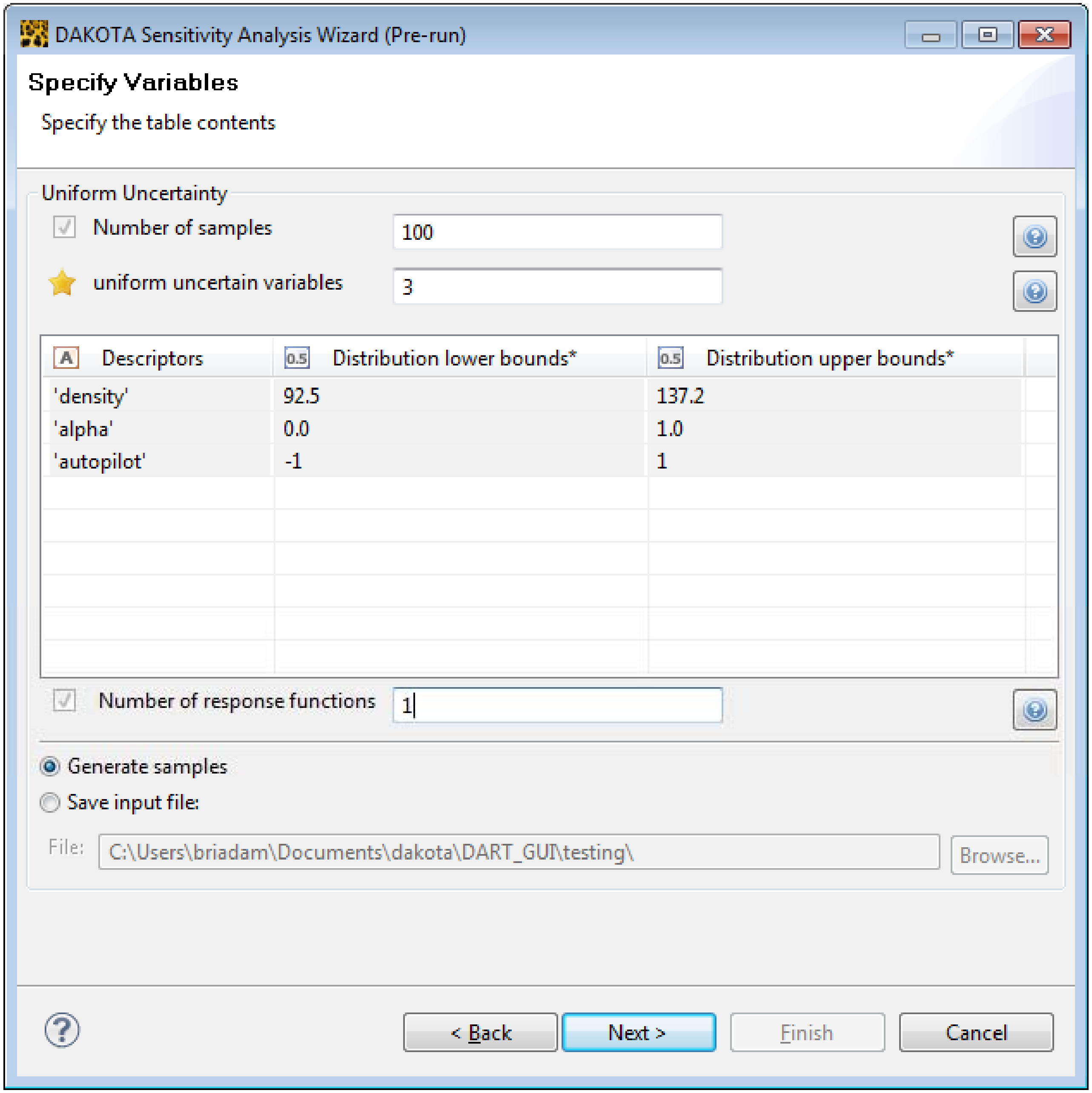
JAGUAR Sensitivity Analysis Wizard



JAGUAR Plans

- Remote job submission to compute clusters
- Integration with DART Workbench
- Better help facilities
- Usability enhancements
- Wizards for creating various kinds of studies

DAKOTA Overview Goals

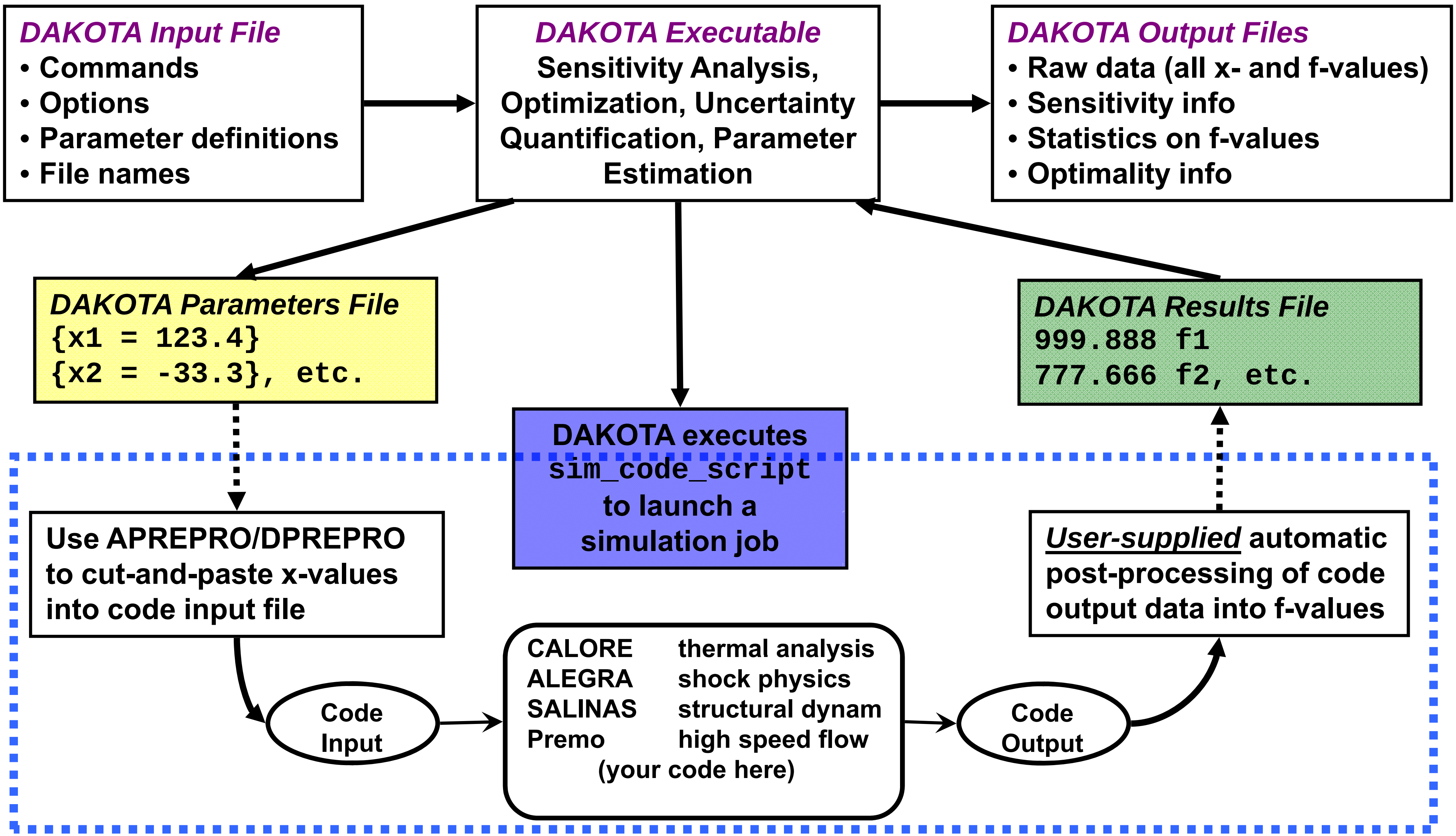
GOAL: Help you decide if DAKOTA might be relevant for your work

- Overview of DAKOTA, key capabilities
- Four categories of methods, with examples
- Getting Started
- *Choose your adventure:*
  - Advanced capabilities (models, parallelism, strategies)
  - JAGUAR graphical user interface
  - Interfacing with DAKOTA (script and library)

DAKOTA plays a key role in

- **risk-informed analysis and design of engineered systems (with structural, thermal, electrical, and other phenomena),**
- **nuclear energy initiatives (including CASL, NEAMS), as well as**
- **product R&D and scientific discovery worldwide.**

DAKOTA (Black-box) Execution & Info Flow



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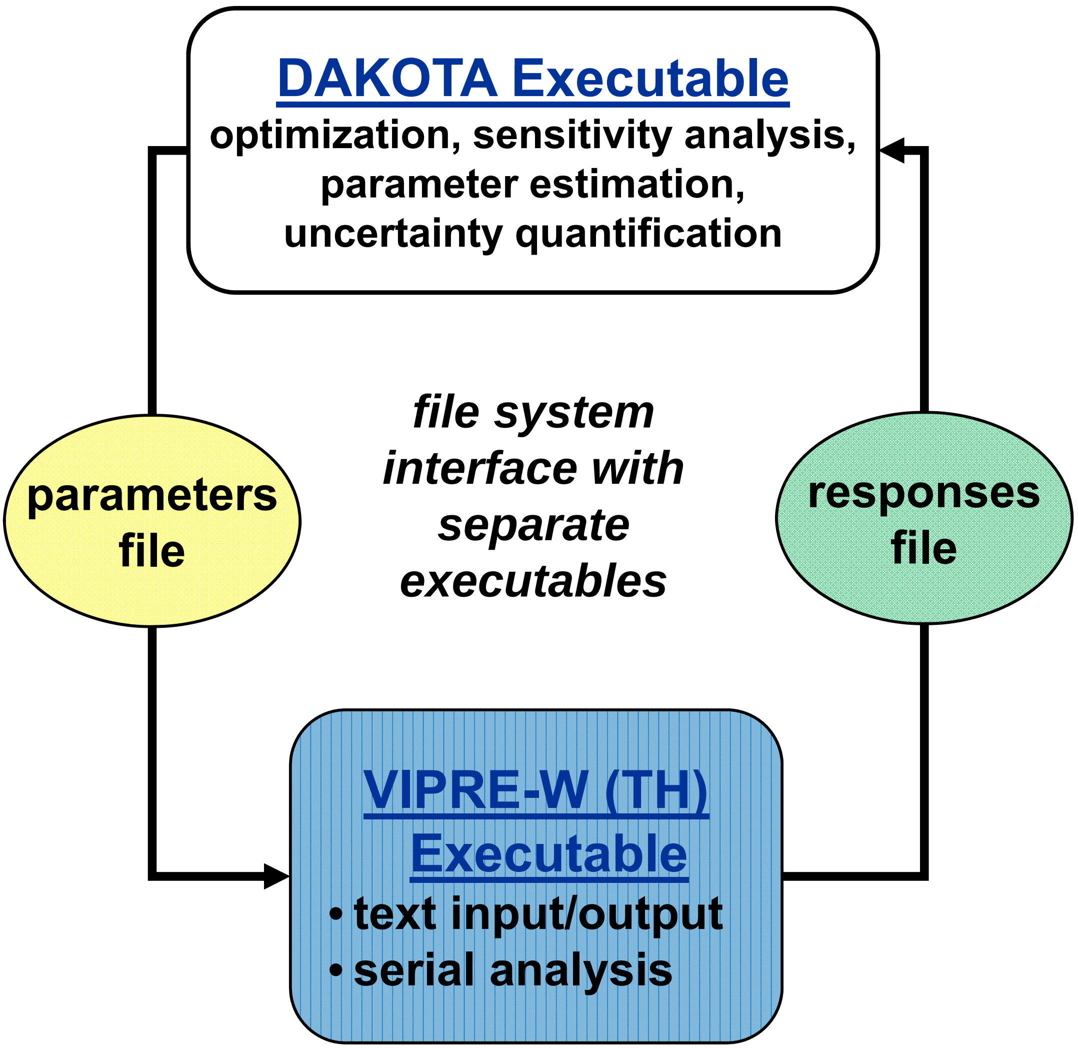
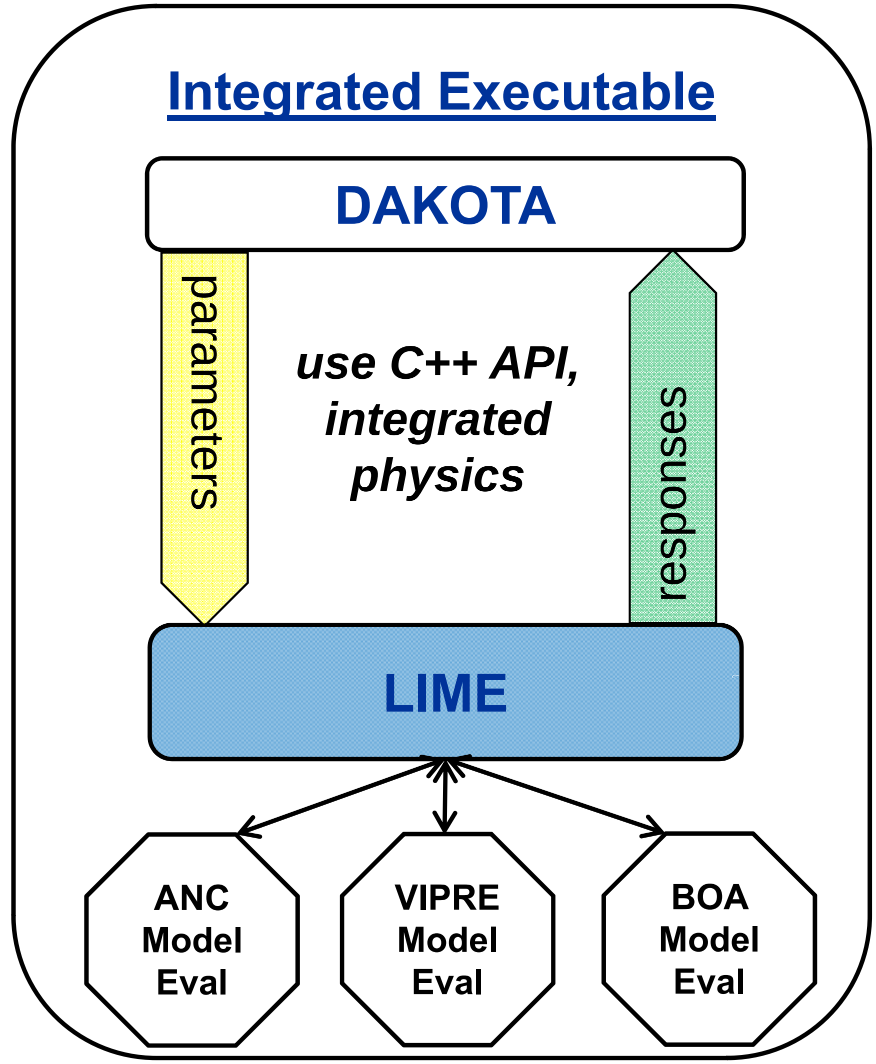
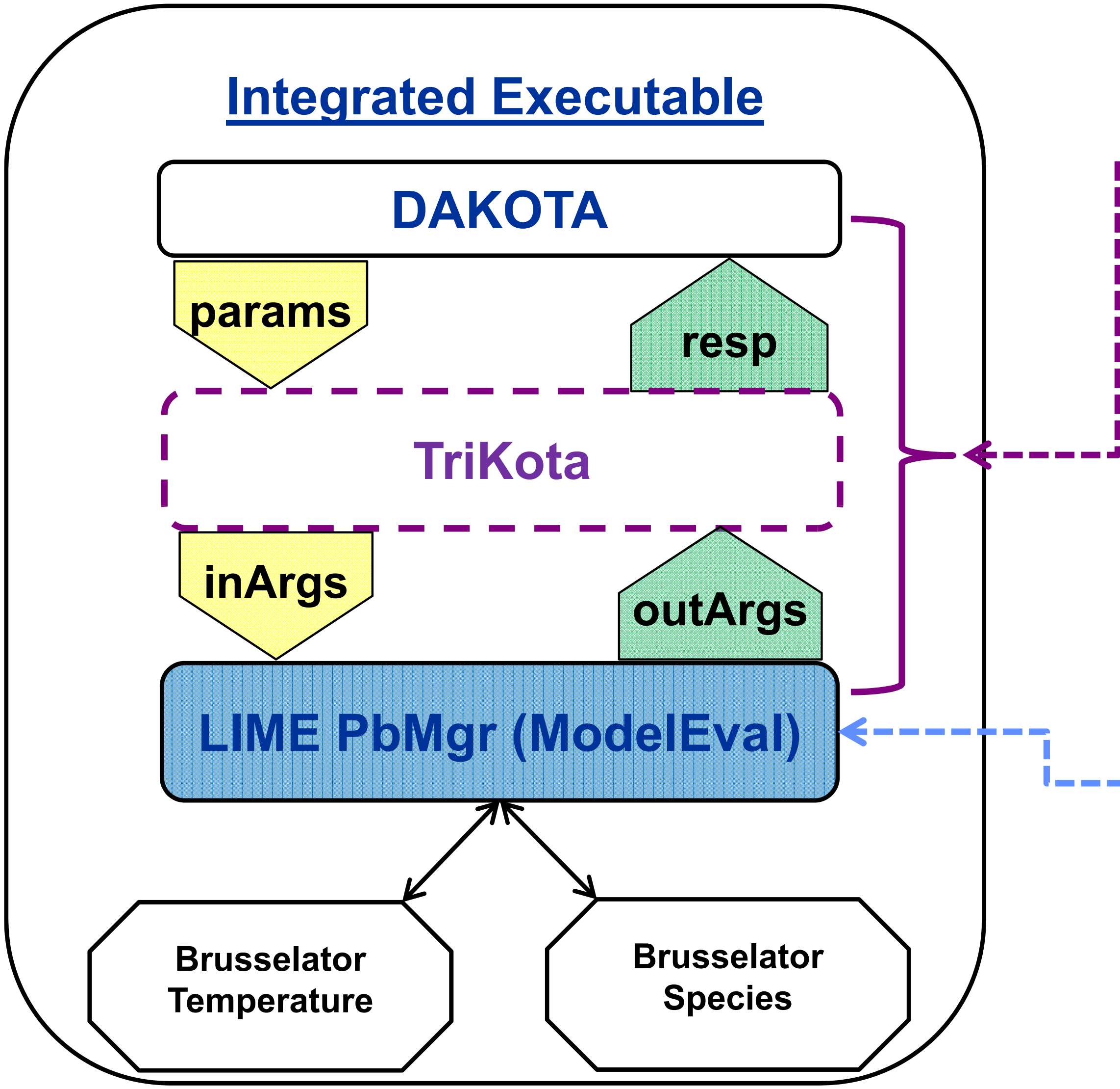
Sample Integrated Executable





TriKota Bridges DAKOTA to LIME



- TriKota (Andy Salinger): lightweight Trilinos package; adapts DAKOTA's parameter/ response API to a Trilinos ModelEvaluator; provides DAKOTA driver
- ModelEvaluator::evalModel maps inArgs (e.g., x, t; p) to outArgs (e.g., g(x, t; p), R(x, t; p)) via Teuchos parameter lists
- LIME problem manager (now) "isa" Model Evaluator; exchange info from DAKOTA to LIME through evalModel(inArgs, outArgs)

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Details: TriKota adapts DAKOTA to ModelEvaluator

TriKota::Driver

- parallel_lib : Dakota::ParallelLibrary
- problem_db : Dakota::ProblemDescDB
- selected_strategy : Dakota::Strategy

- run(Dakota::DirectApplicInterface *)
- getFinalSolution() : Dakota::Variables

Driver abstracts away complexity of managing DAKOTA library mode

DAKOTA:: DirectApplicInterface

- *dakota_params*
- *dakota_responses*

- *derived_map_ac()*

TriKota:: DirectApplicInterface

- model_params
- model_responses
- model_gradients

- derived_map_ac()

Key: modified LIME ProblemManager so it "isa" ModelEvaluator and can be registered with this interface. Hence, DAKOTA's map calls LIME

App : EpetraExt:: ModelEvaluator, e.g., LIME Problem Manager

Enables easy configuration: pseudocode example

```
TriKota::Driver dakota;

LIME::ProblemManager pm;
// ...configure pm to run Brusselator
// (set XML, register physics modules)

// register LIME with dakota and run
TriKota::DirectApplicInterface
  trikota_interface(dakota.db(), pm);
dakota.run(trikota_interface);
```

Getting Started with DAKOTA

- Access a supported installation (preferred) or download the software from DAKOTA webpage
- Attend a DAKOTA training class
- User's Manual, Chapter 2: Tutorial, corresponding examples distributed with DAKOTA
- Support:
  - User forum: `dakota-users@software.sandia.gov` (DAKOTA team and internal/external user community)
  - All support options: `http://dakota.sandia.gov/resources.html`

Thank you for your attention!

`http://dakota.sandia.gov/`

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Abstract

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DAKOTA Overview and Application Examples

DAKOTA is a freely available software package for sensitivity analysis, optimization, uncertainty quantification, and calibration with black-box computational models (simulations). DAKOTA provides a flexible, extensible interface to any analysis code, includes both established and research algorithms designed to handle challenges with science and engineering models, and manages parallelism for concurrent simulations. DAKOTA strategies support mixed deterministic/probabilistic analyses. This overview will survey the classes of methods in DAKOTA, offer application examples, and describe interfaces both to DAKOTA and between DAKOTA and simulation codes.