SAND2010-6199P

DAKOTA Capability Overview

CASL/VRI Workshop, August 26, 2010

Brian Adams, **DAKOTA Project Lead**
Optimization and Uncertainty Quantification

- **DAKOTA capabilities enabling V&V / UQ**
  - **Overview, key capabilities**
  - **Four categories of methods: SA, UQ, *optimization, calibration***
  - **Advanced capabilities**
- **Usability vision: JAGUAR GUI, library interface**

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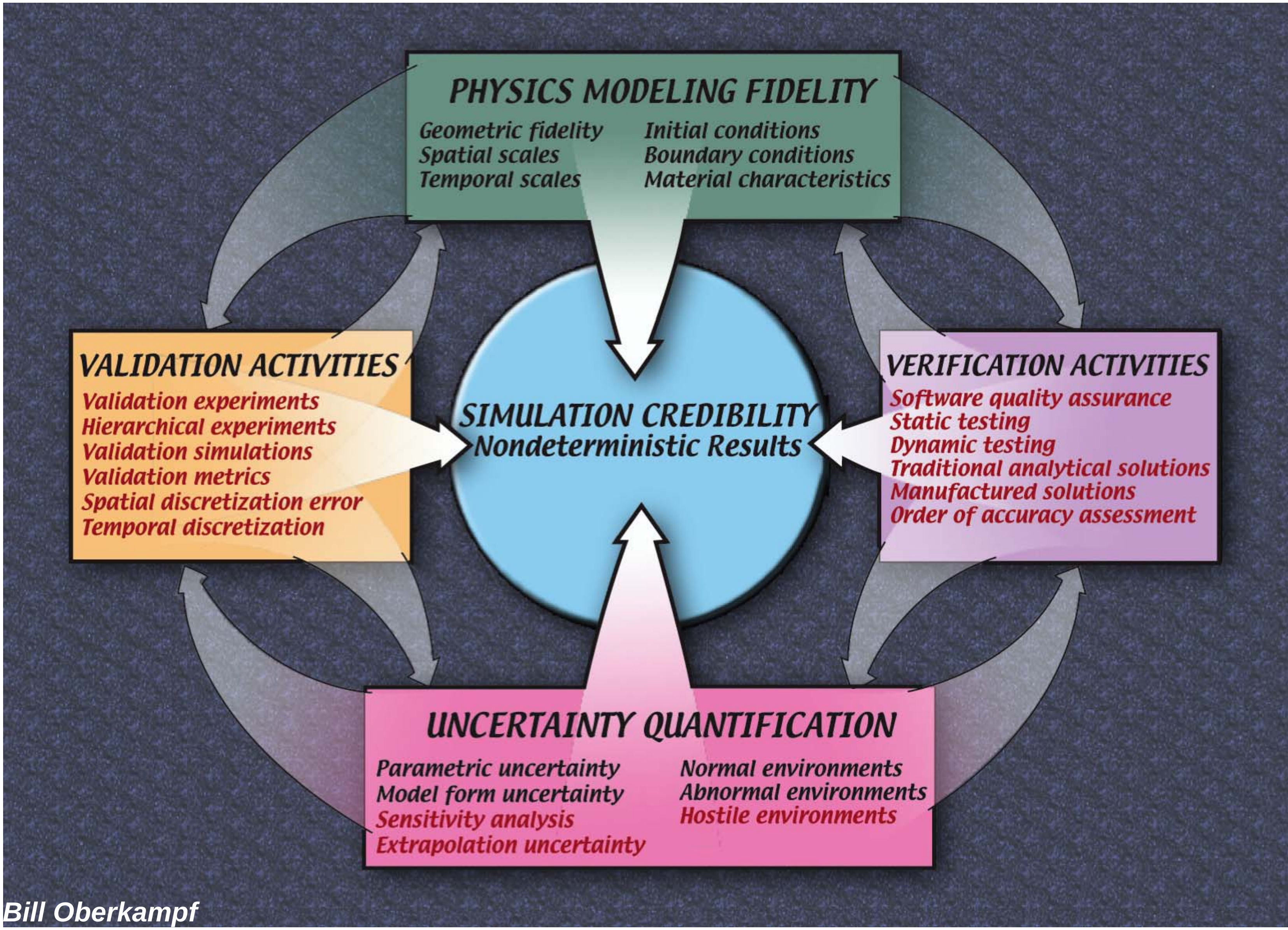
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

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

Ultimate purpose (arguably): insight, prediction, and risk-informed decision-making → *need credibility for intended application*



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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***

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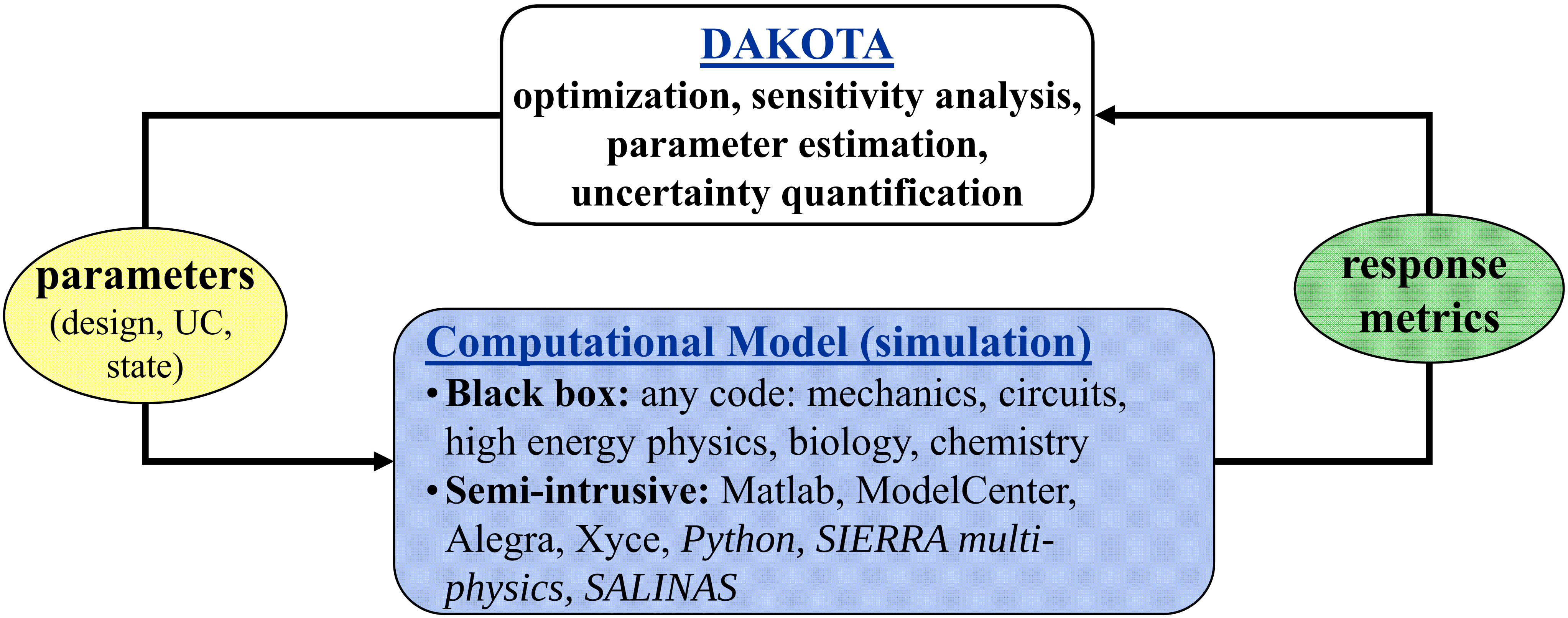
Automated Iterative Analysis

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)

Sample Applications with INL

DAKOTA+R7 Analyses

- **Sensitivity Analysis: what variables influence reactor performance measures, e.g., peak coolant temperature (PCT)?**
- **Uncertainty Quantification: what are mean, s.d., distribution of a response (PCT), given distributions on input parameters: pump power lost, SCRAM delay, control rod injection distance, etc.?**
- **Design optimization: What geometries, fuel configuration, operation maximize power, minimize cost, and are "robust"?**

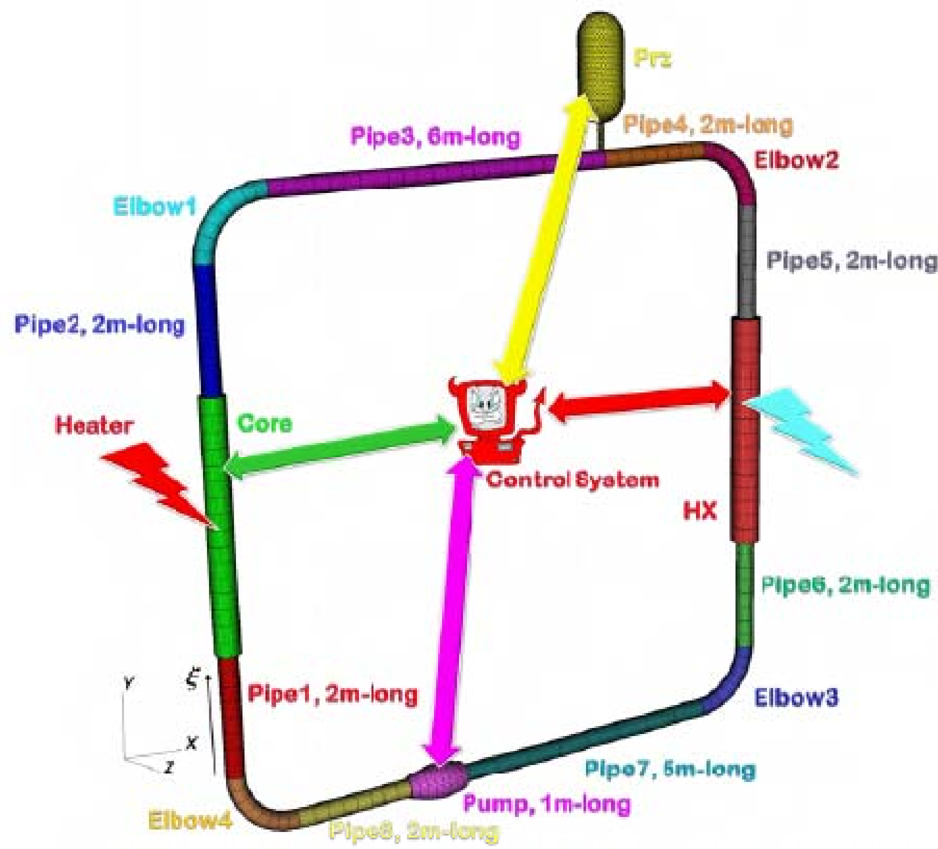


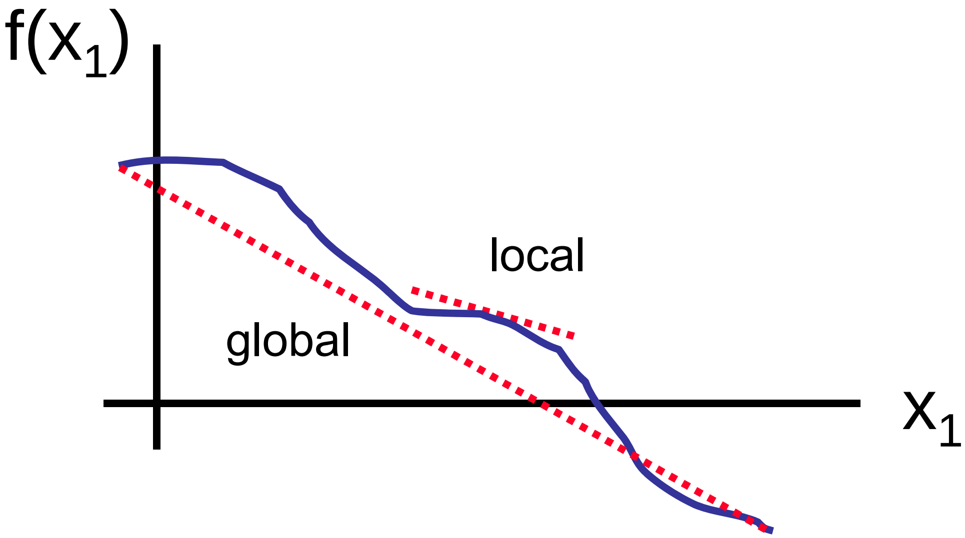
Fig. A.29: Formulation of the "VR_2" reactor problem.

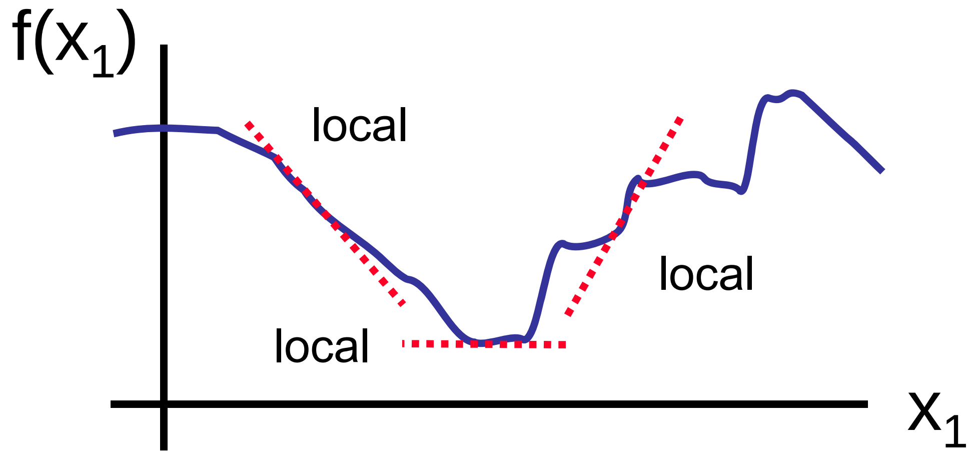
DAKOTA+Eranos Analyses

- **Sensitivity Analysis: sensitivity of neutronics with local and global SA methods**
- **Large analysis: looked at various energy group/species correlation with outputs such as Keff**

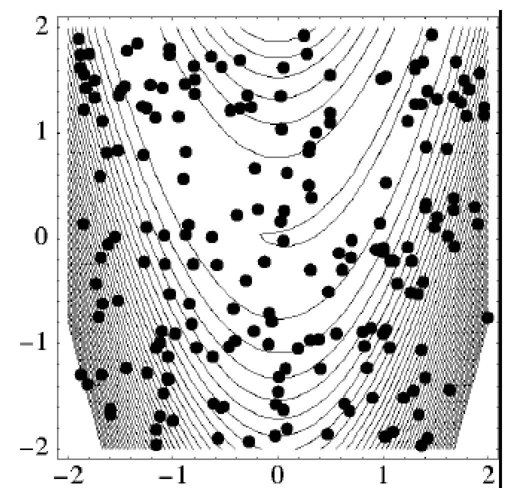
Sensitivity Analysis

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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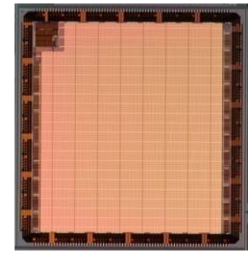
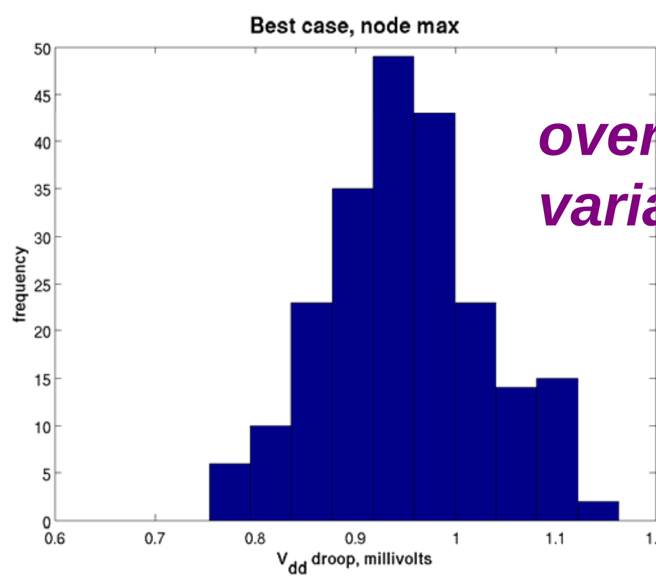
SA for Electrical Circuits

- **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)**



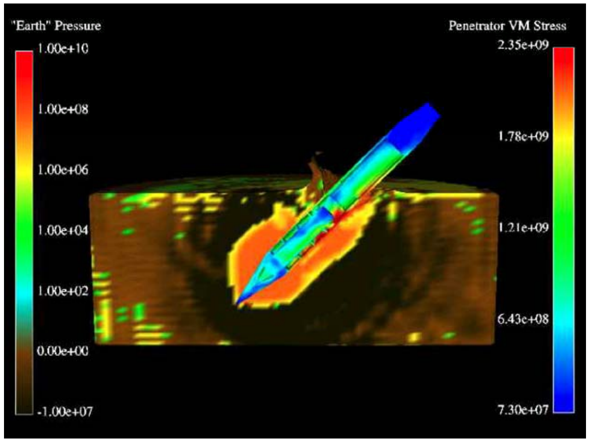
	Vdd Metrics	
	node max	node avg
METAL1	0.96	0.82
METAL2	0.11	0.04
METAL3	0.10	0.05
METAL4	0.80	0.81
METAL5	0.86	0.91
VIA1	0.71	0.66
VIA2	0.80	0.76
VIA3	0.57	0.60
VIA4	0.91	0.94
CONTACT	0.21	0.13
polyc	0.04	0.05

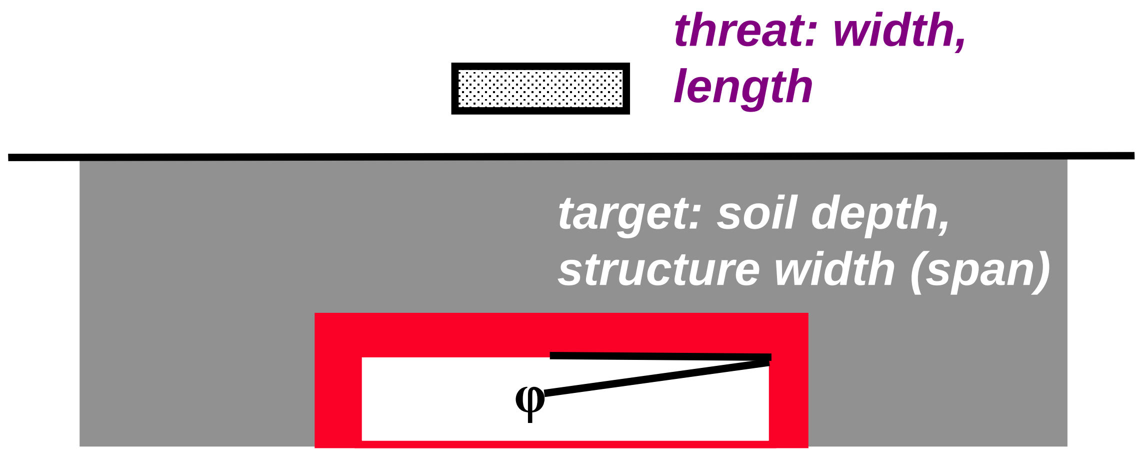
correlations



overall variability

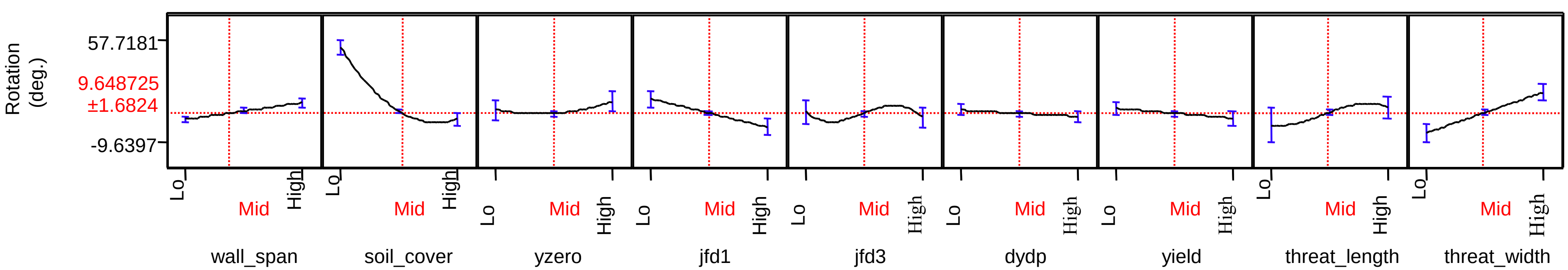
SA of Penetrator





Notional model for illustration purposes only (http://www.sandia.gov/ASC/library/fullsize/penetrator.html)

- **Underground target with external threat: assess uncertainty in target response given uncertainty in target construction and threat characteristics**
- **12 parameters describing target & threat uncertainty**
- **Response: angular rotation (φ) of target roof at mid-span**
- **Analysis: CTH Eulerian shock physics code; JMP stats**



DAKOTA Sensitivity Analysis

- **Parameter study, design and analysis of computer experiments, and general sampling methods:**
  - **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 (derivative-based)**

- **DAKOTA outputs basic statistics on responses, including mean, standard deviation, and correlations; tabular output can be analyzed with any third-party statistics package**
- **Determine main effects and key parameter *interactions***
- **In SA, one typically does not make a distribution assumption**

Uncertainty Quantification

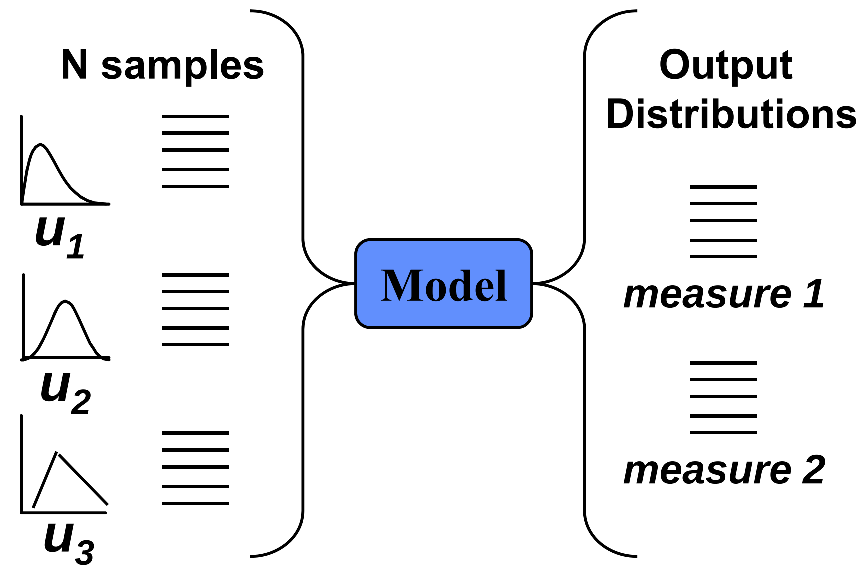
Forward propagation: quantify the effect that uncertain (nondeterministic) input variables have on model output

<u>Input Variables *u*</u> **(physics parameters, geometry, initial and boundary conditions)** → **Computational Model** → **Variable Performance Measures *f(u)***

(possibly given distributions)

Potential Goals:

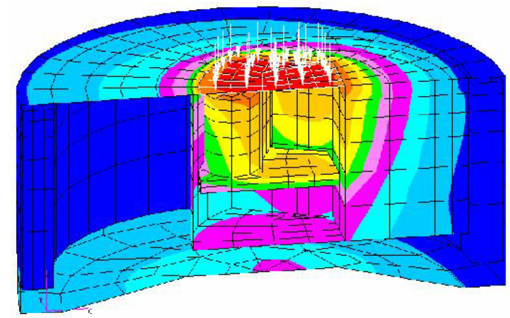
- **based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)**
- **identify parameter correlations/local sensitivities, robust optima**
- **identify inputs whose variances contribute most to output variance (global sensitivity analysis)**
- **quantify uncertainty when using calibrated model to predict**

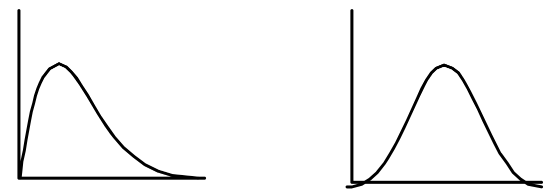


Typical method: Monte Carlo Sampling

Thermal
Uncertainty Quantification

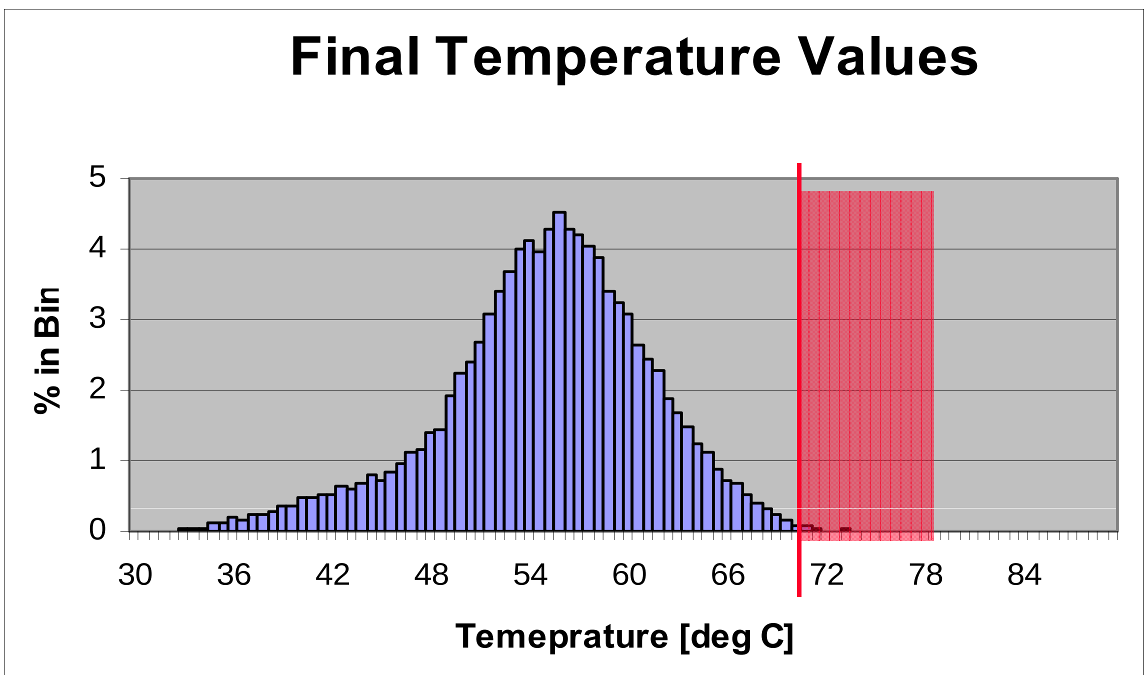
- **Device subject to heating** **(experiment or computational simulation)**
- **Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by** $u_1, \ldots, u_N$
- **Response temperature** $f(u)=T(u_1, \ldots, u_N)$ **calculated by heat transfer code**



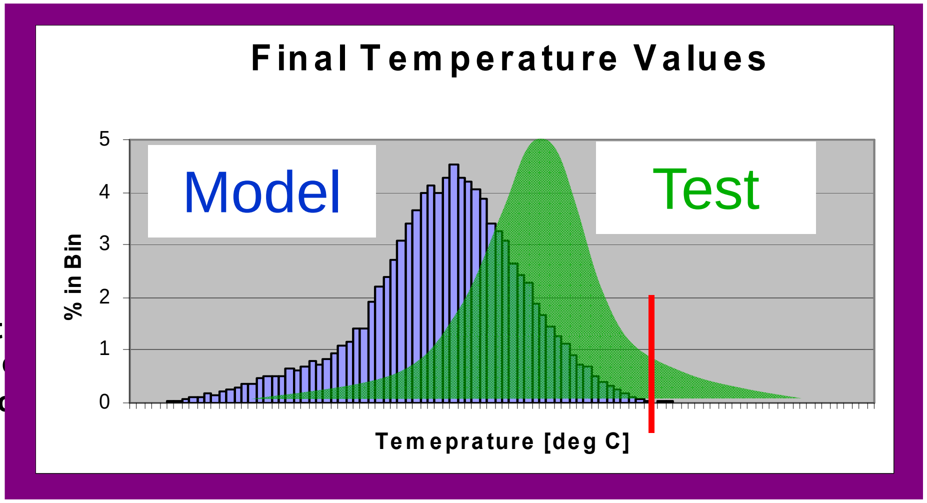


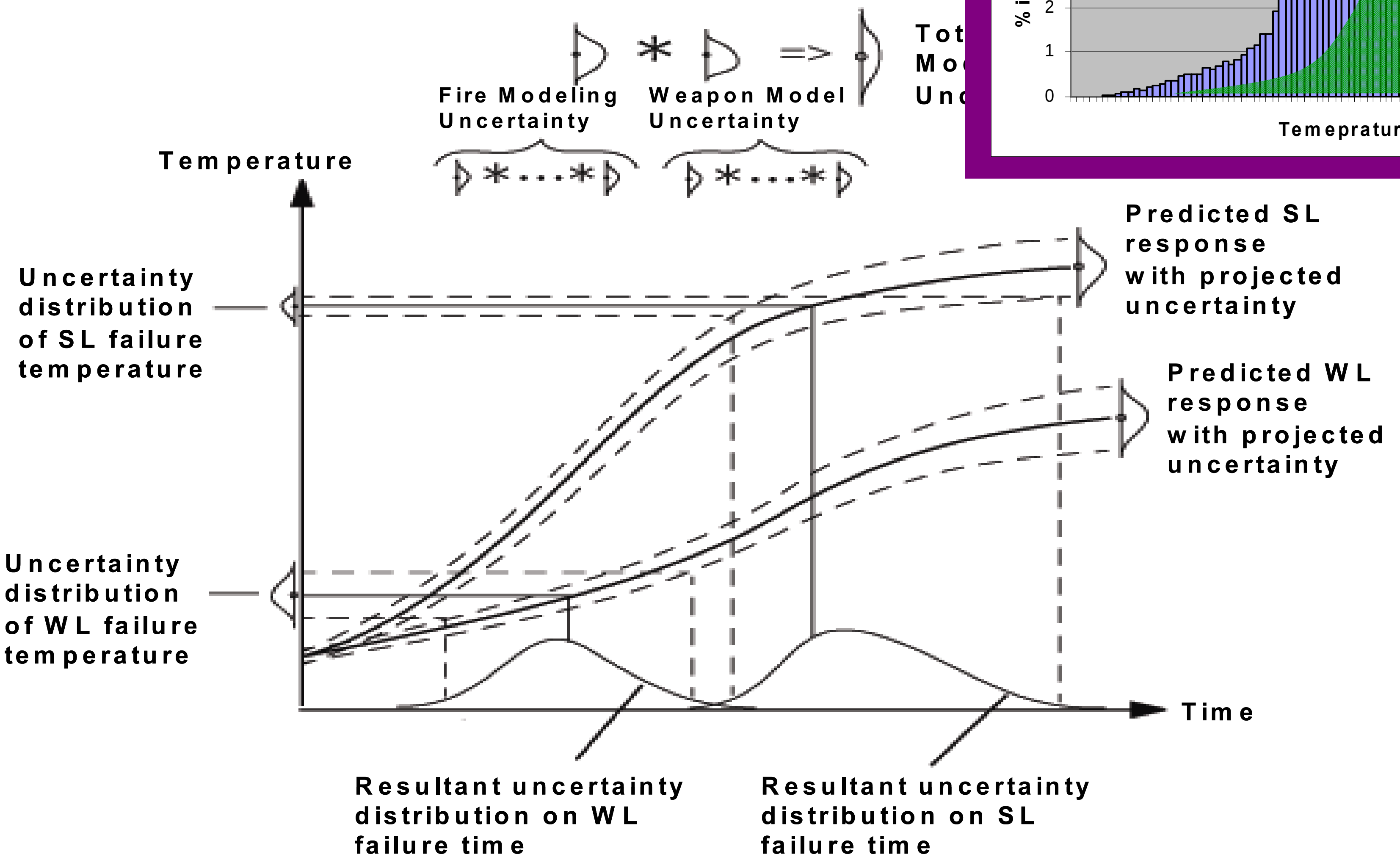
Given distributions of $u_1,\ldots,u_N$***, UQ methods calculate statistical info on outputs:***

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



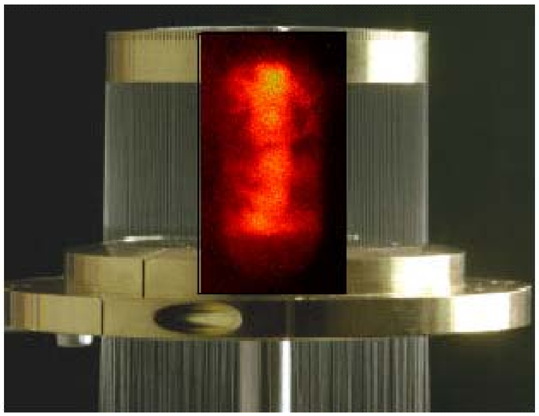
UQ for Thermal Race



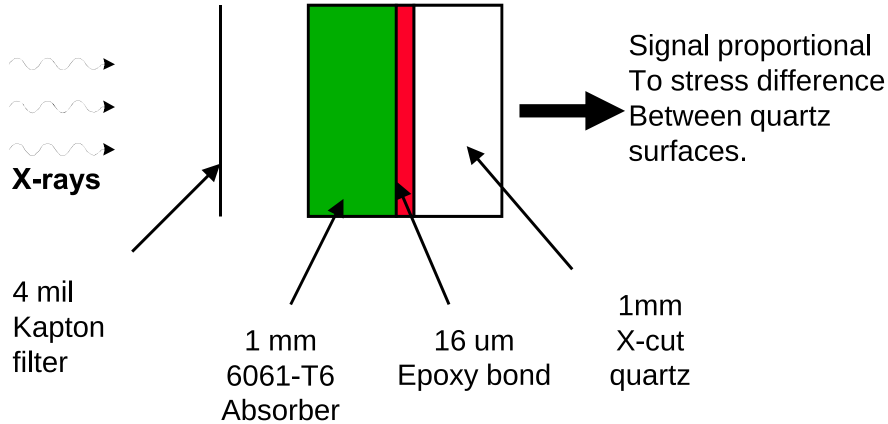


UQ for Validation: Presto Simulations vs. Z-Accelerator Data

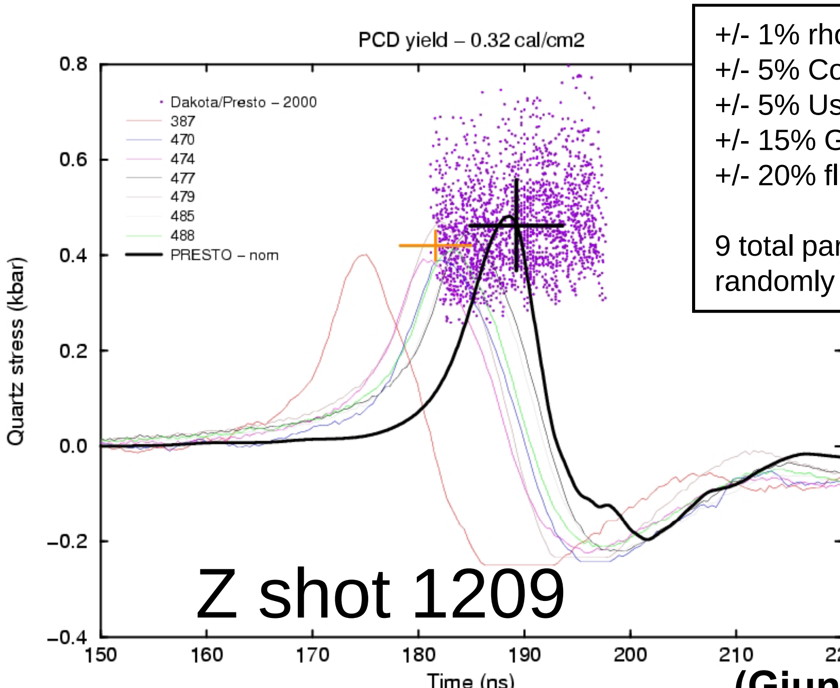
Tungsten wire array & Z pinch



X-Ray Induced Thermomechanical Shock Modeled w/ Presto

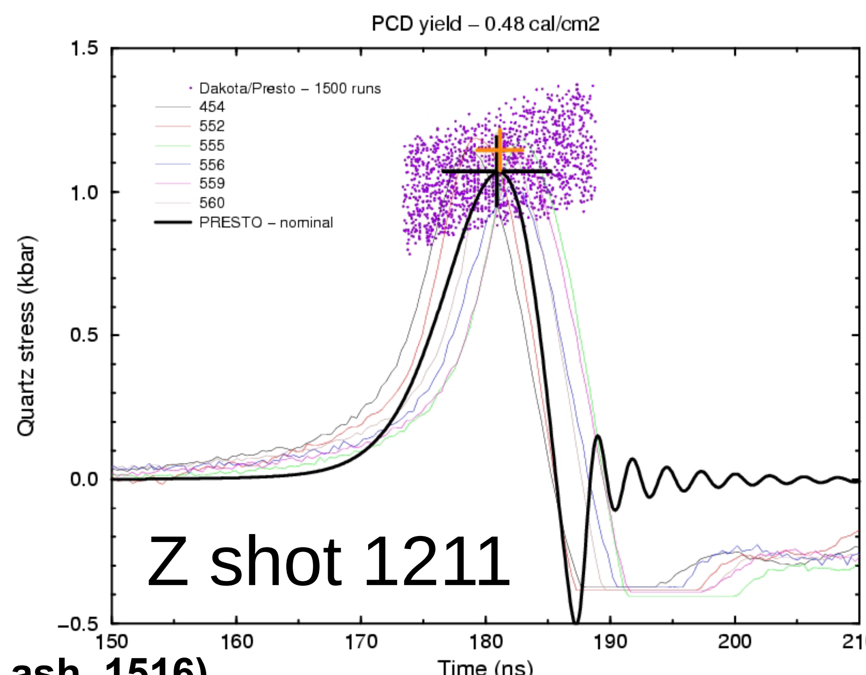


- **UQ study on Presto thermomechanical shock**
- **DAKOTA+Presto, 2000 runs; on distributed network of workstations**
- **Compared Presto vs. Z Shot μ±1σ uncertainty**
- **UQ study gave info on design margins; identified need for model improvement**



+/- 1% rho
+/- 5% Co
+/- 5% Us/Up slope
+/- 15% Gruneisen
+/- 20% fluence

9 total parameters randomly varied



(Giunta, 1544; Lash, 1516)

DAKOTA UQ:
You can do better than Monte Carlo!

- **Techniques for propagating aleatory uncertainty (variables characterized by probability distributions) through models:**
  - **Latin hypercube (and other Monte Carlo) sampling**
  - **Local reliability methods (mean value, MPP search, FORM, SORM)**
  - **Global reliability methods (EGRA)**
  - **Non-intrusive stochastic expansion methods (polynomial chaos and stochastic collocation)**

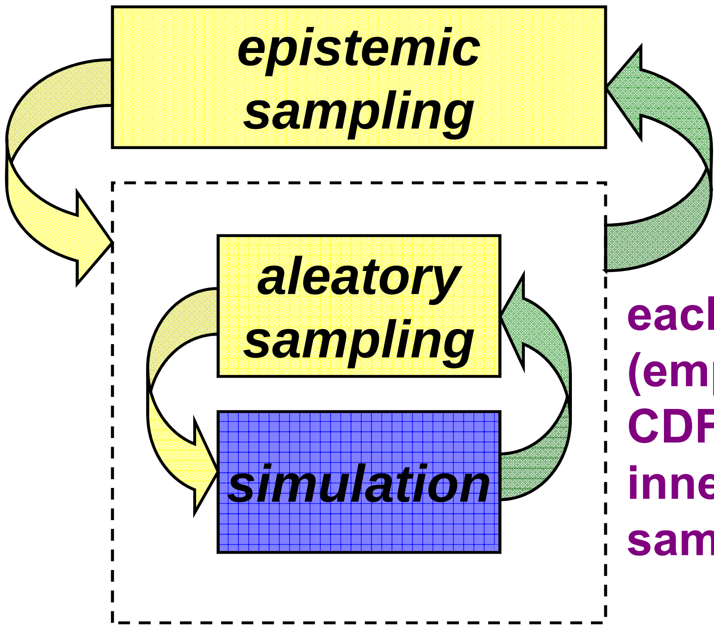
- **Methods for epistemic uncertainty (variables characterized by intervals or basic probability assignments):**
  - **Local/global interval estimation**
  - **Local/global Dempster-Shafer evidence theory (belief/plausibility)**
  - **"Second-order" probability**

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

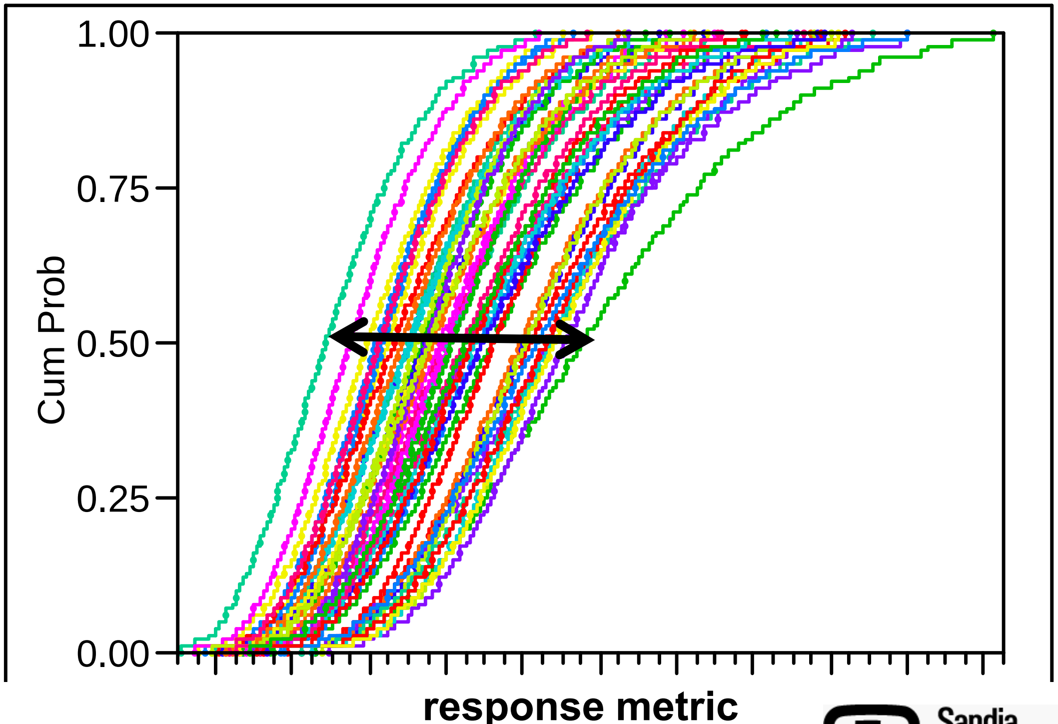
"Second-Order" Probability

- **Nested sampling technique frequently used in QMU studies**
- **For each outer loop sample of epistemic (interval) variables, run an inner loop UQ study over aleatory (probability) variables**
- **Example: Radiation Transport milestone studies:** Uncertainties in materials, energies, incoming radiation characteristics → determine uncertainty range on output measures like current or voltage and if requirements met

50 outer loop samples → 50 CDF traces



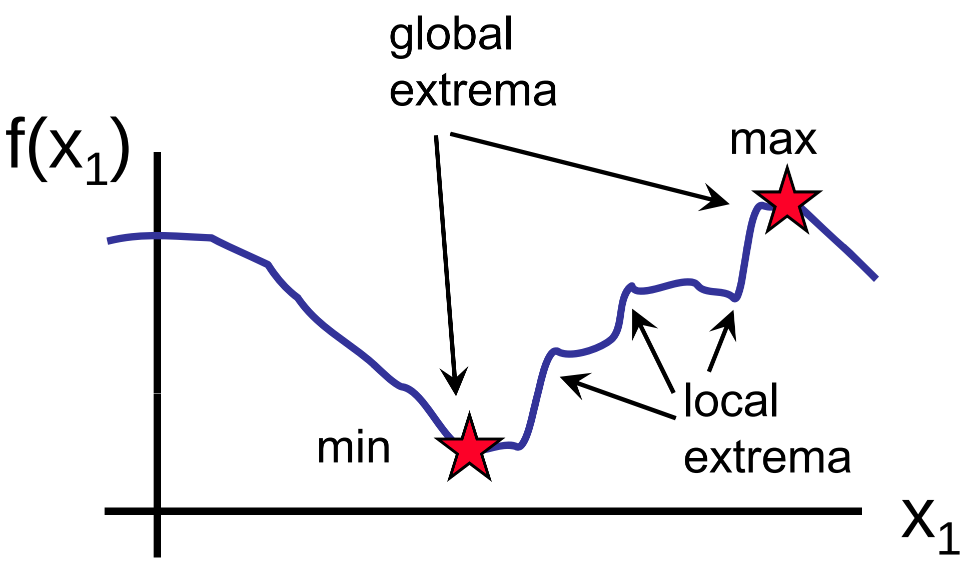
each discrete (empirical) CDF: 100 inner loop samples



"Envelope" of CDF traces represents response epistemic uncertainty

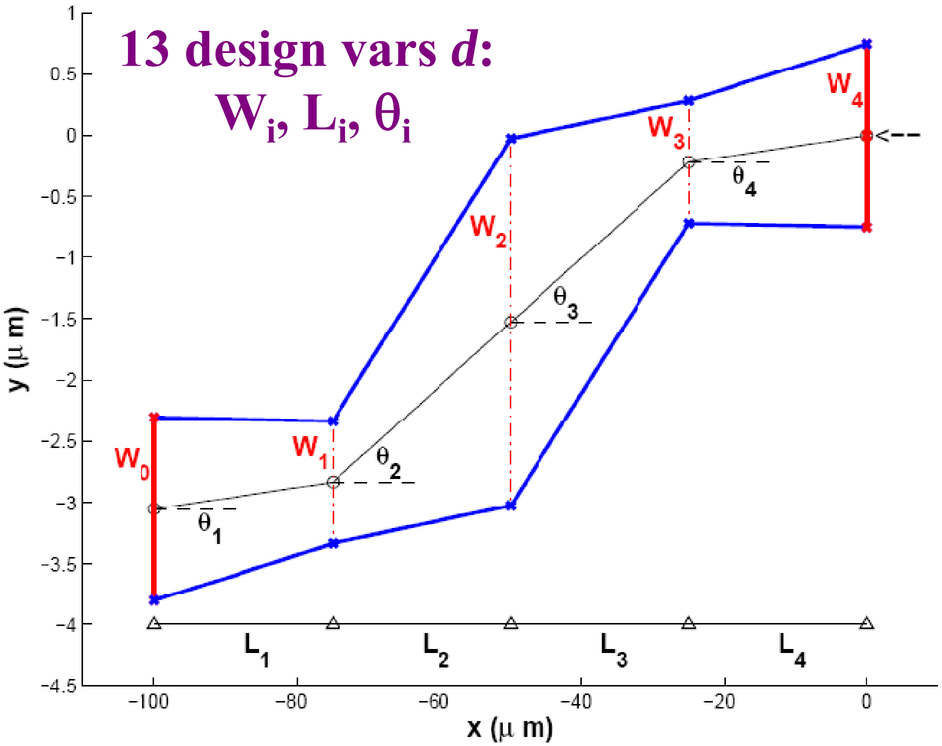
Nonlinear Optimization

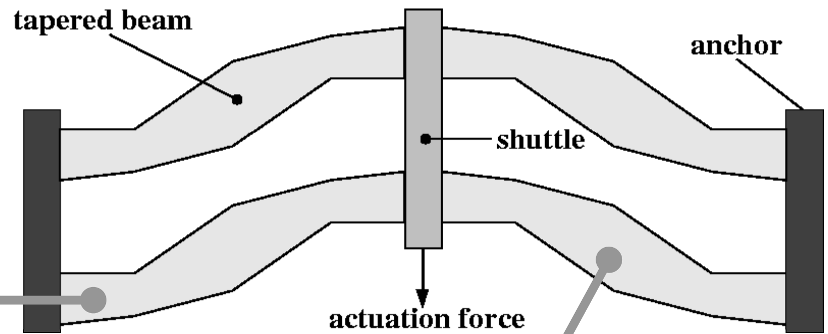
- GOAL: Vary parameters to extremize objectives, while satisfying constraints to find (or tune) the best design, estimate best parameters, analyze worst-case surety, e.g., determine:
  - delivery network that maximizes profit while minimizing environmental impact
  - case geometry that minimizes drag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

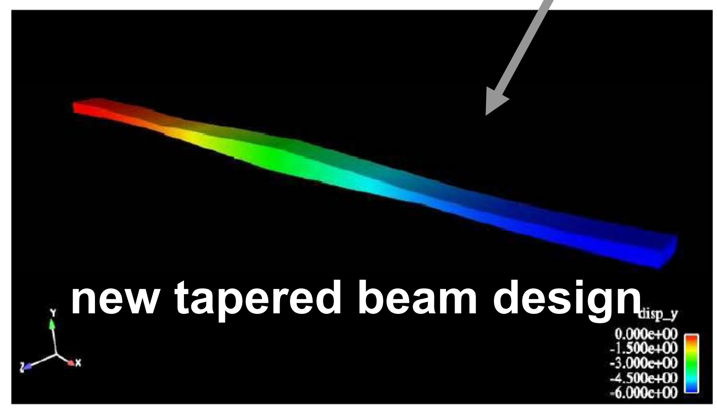


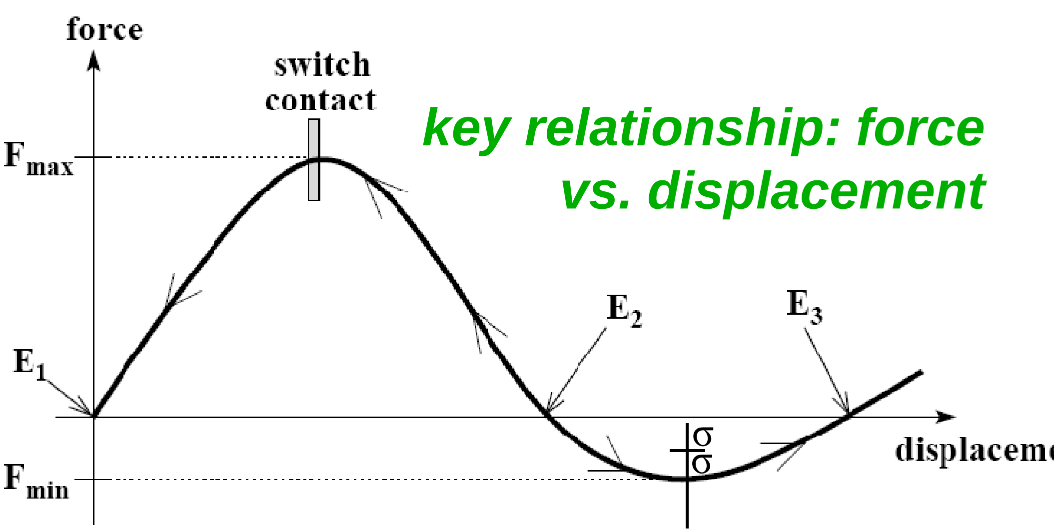
Some applications: local improvement suffices; others: must find global minimum at any cost

MEMS Switch Design: Geometry Optimization







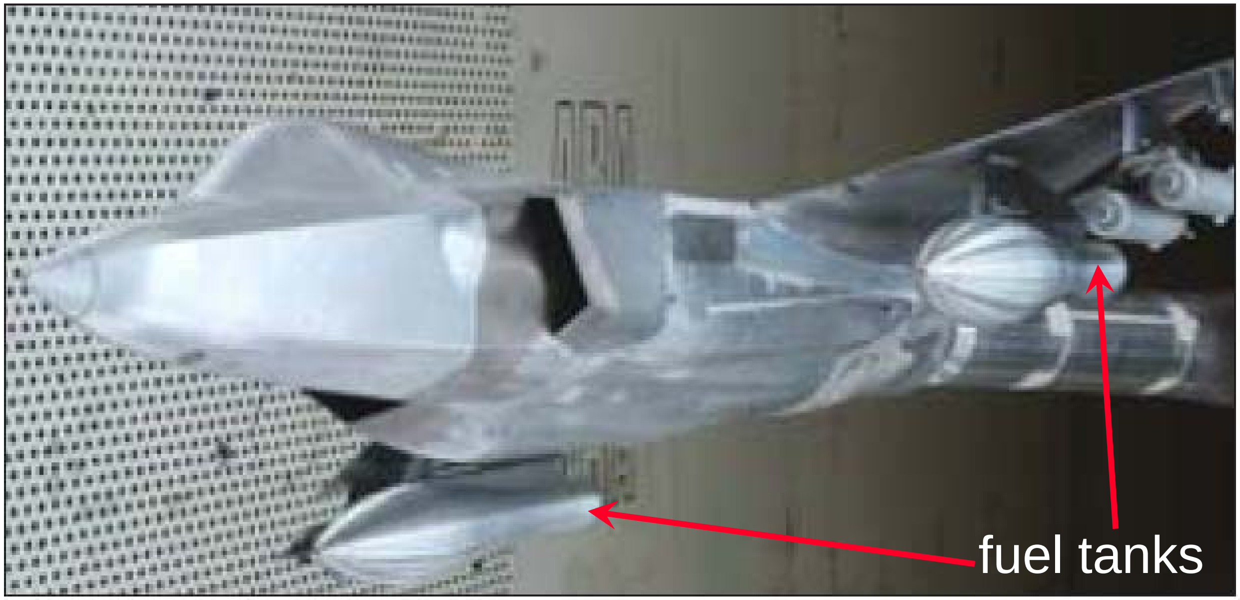


key relationship: force vs. displacement

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**

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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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)***

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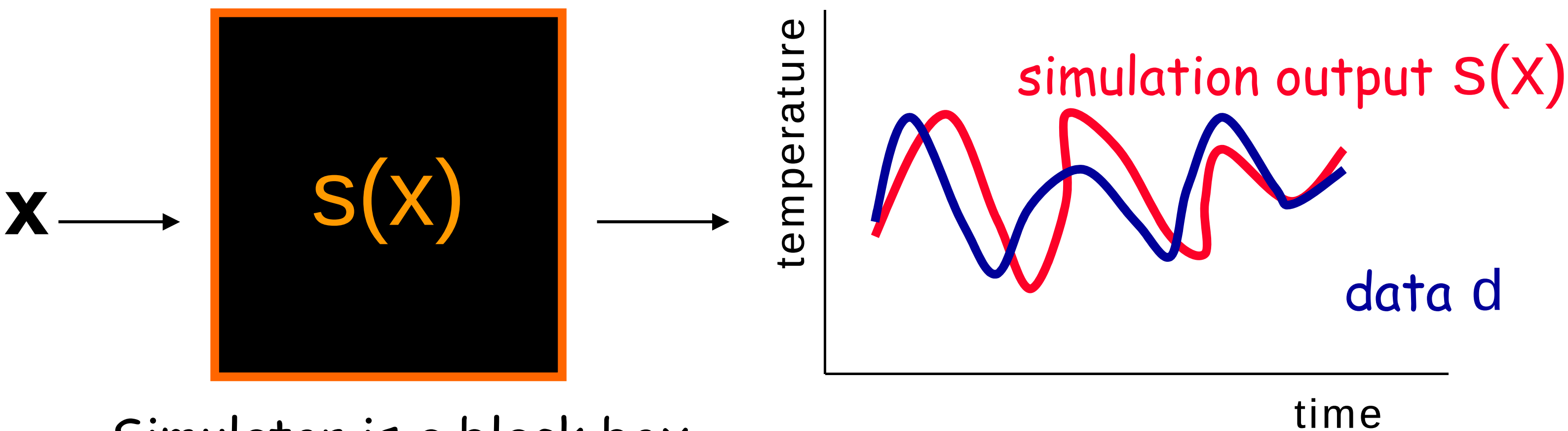
Calibration/Parameter Estimation

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

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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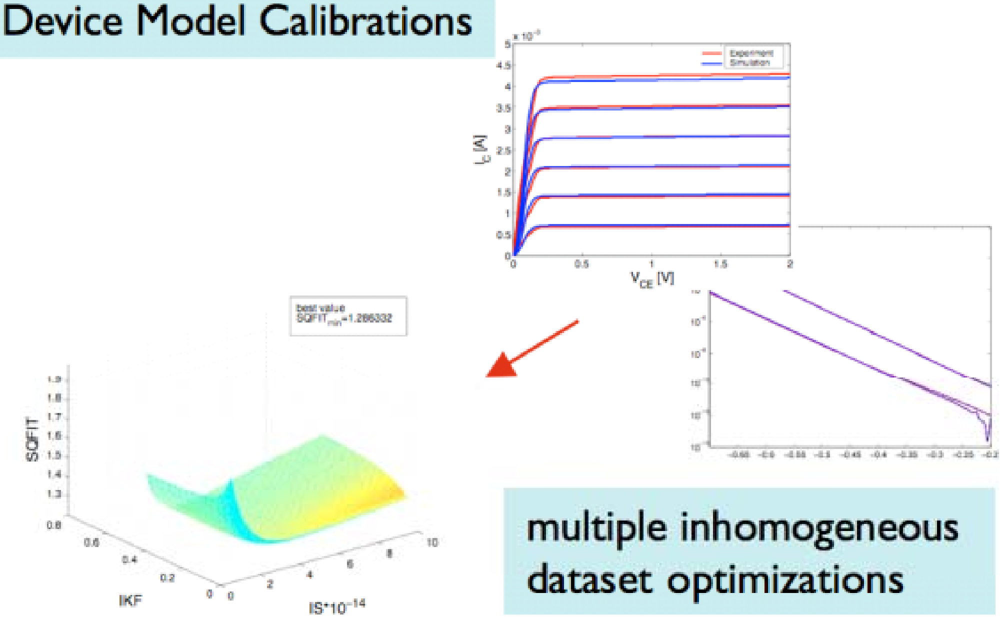
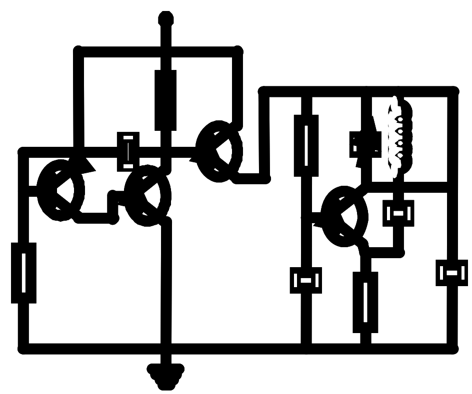
QASPR Model Calibration

- **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

Device Model Calibrations



multiple inhomogeneous dataset optimizations



Flexibility with Models

DAKOTA <u>models</u> 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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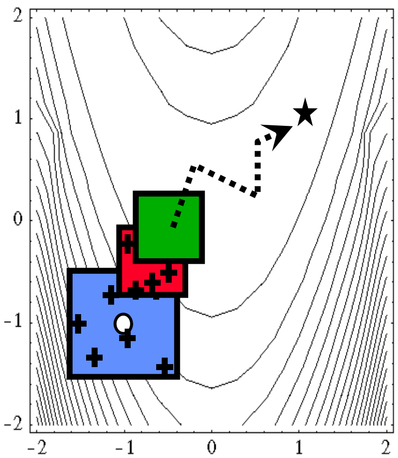
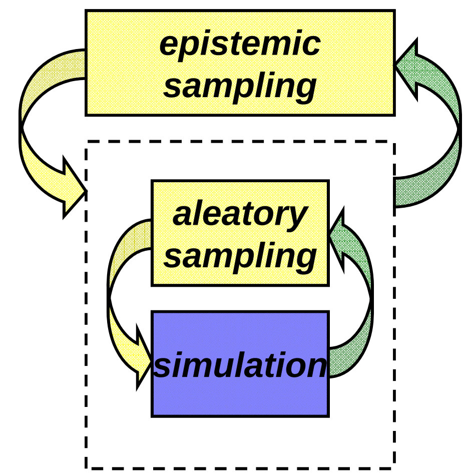
Strategies
(and advanced/multi-component methods)



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

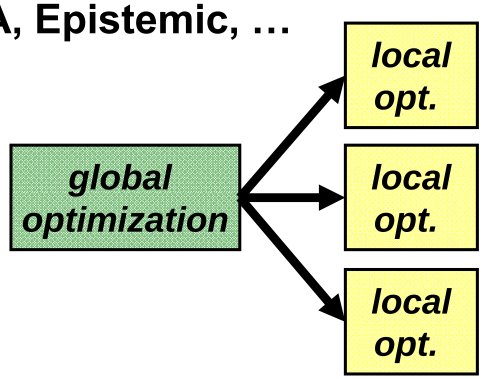
- **opt within opt (multilevel opt & hierarchical MDO)**
- **UQ within UQ (second-order probability)**
- **UQ within opt (OUU) and NLS (MCUU)**
- **opt within UQ (uncertainty of optima)**

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**

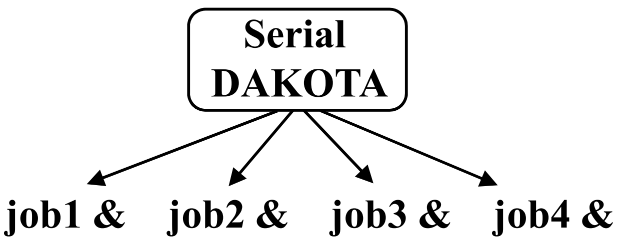
Nonlinear least squares

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

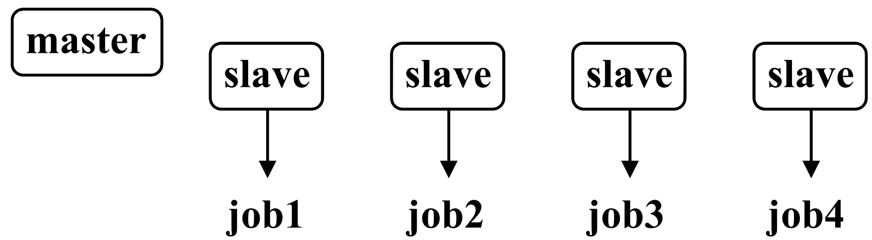
Scalable Parallelism

Nested parallel models support large-scale applications and architectures.

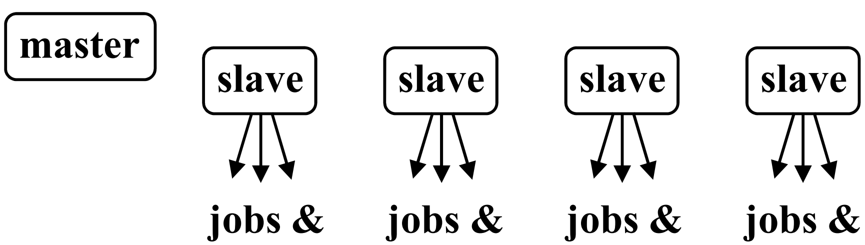
1. SMP/multiprocessor workstations: Asynchronous (external job allocation)



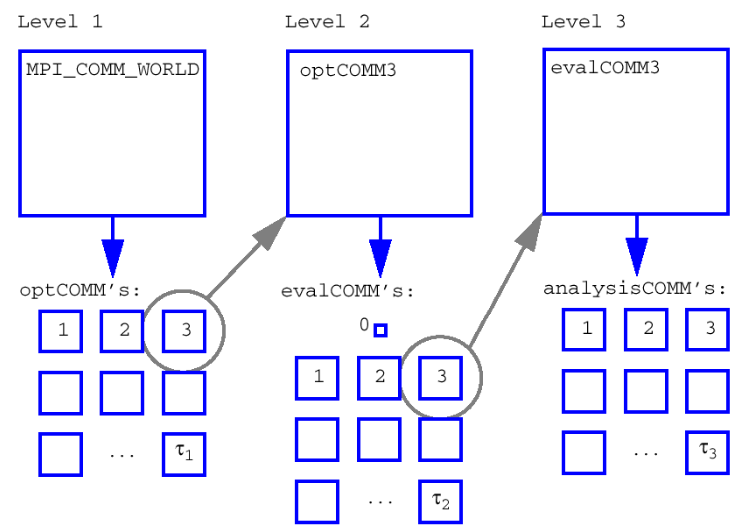
2. Cluster of workstations: Message-passing (internal job allocation)



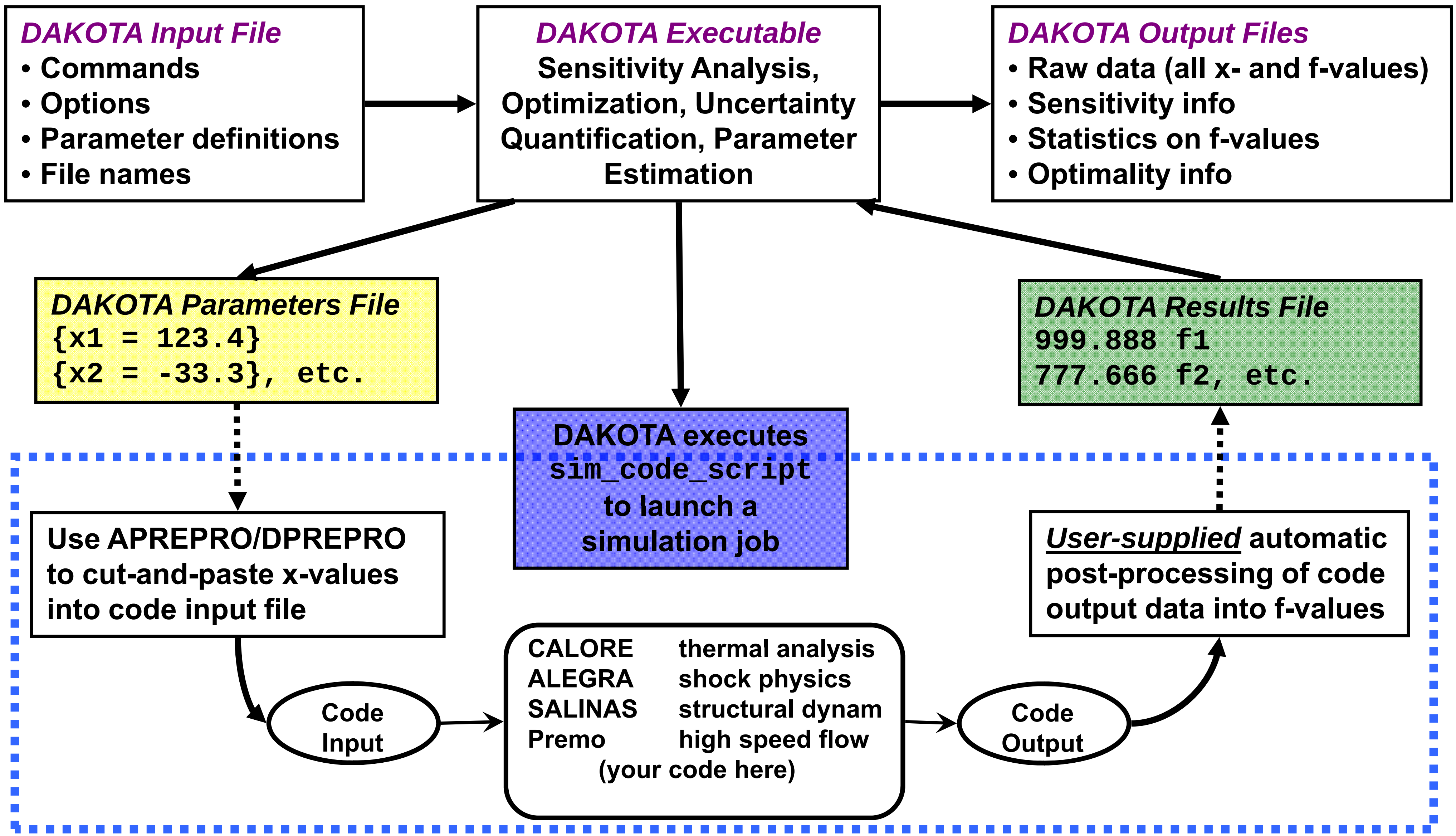
3. Cluster of SMP's: Hybrid (service/compute model)



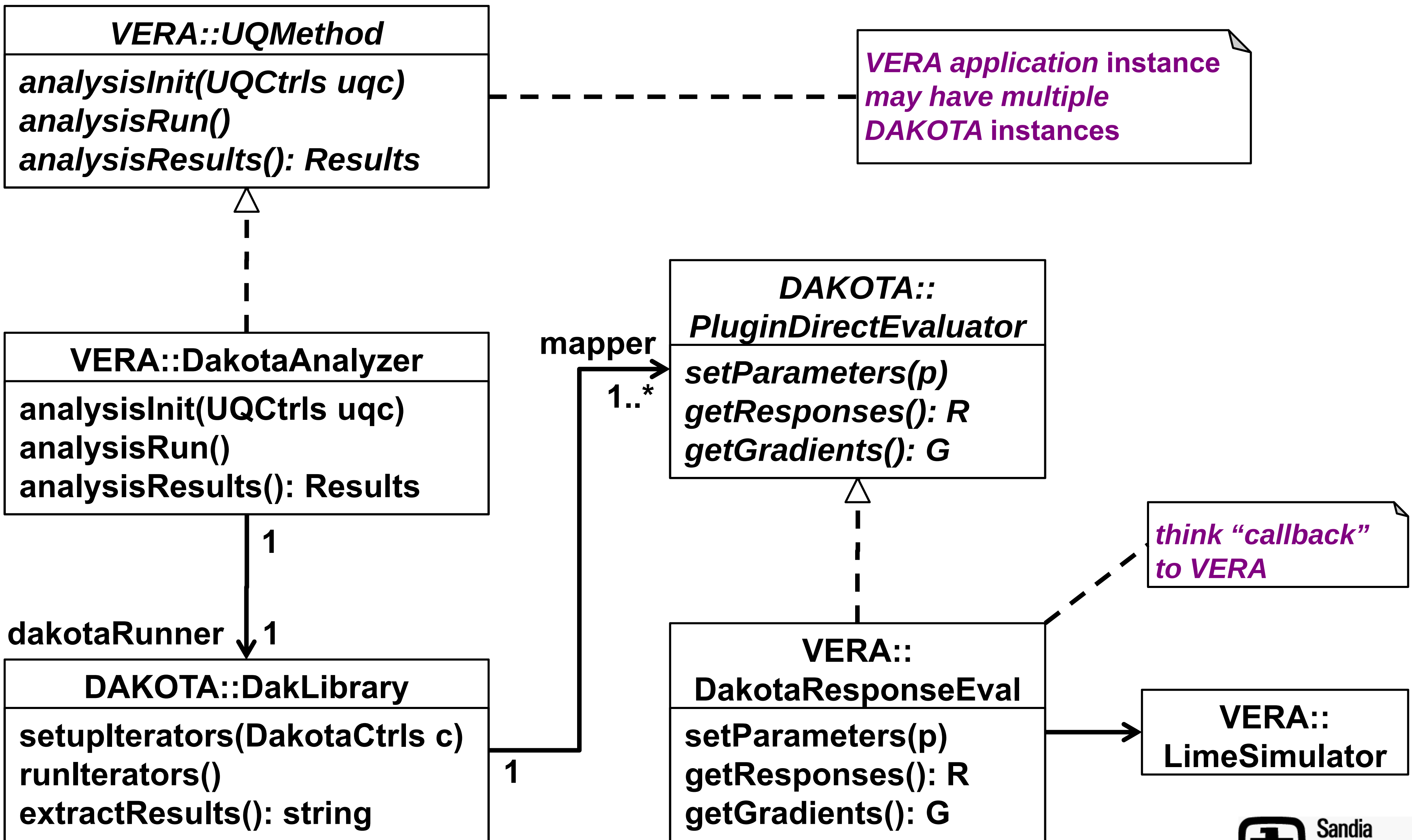
4. MPP (Red Storm/ White): Internal MPI partitions (nested parallelism)



DAKOTA Standalone (Black-box) Execution & Info Flow



Example VERA/DAKOTA Library Interface Structure



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JAGUAR 2.0

- 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 Plans

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

DAKOTA Summary

Sensitivity analysis, uncertainty quantification, optimization, calibration with:

- **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**
- **Scalable parallel computations on clusters**
- **Object-oriented code; modern software quality practices**

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

Bonus Slides

DAKOTA Team

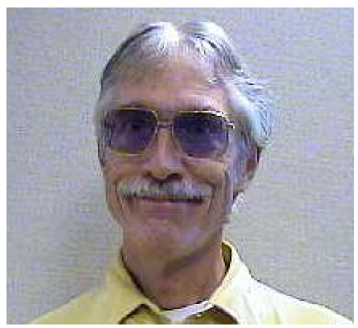
Brian Adams
Project Lead
1411

Mike Eldred
Research Mgr.
1411

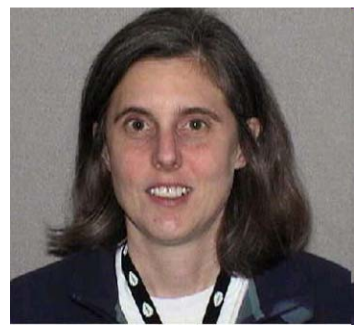
Bill Bohnhoff
Support Mgr.
1341

Jim Stewart
Business Mgr.
1411

Keith Dalbey
1411



Dave Gay
1411

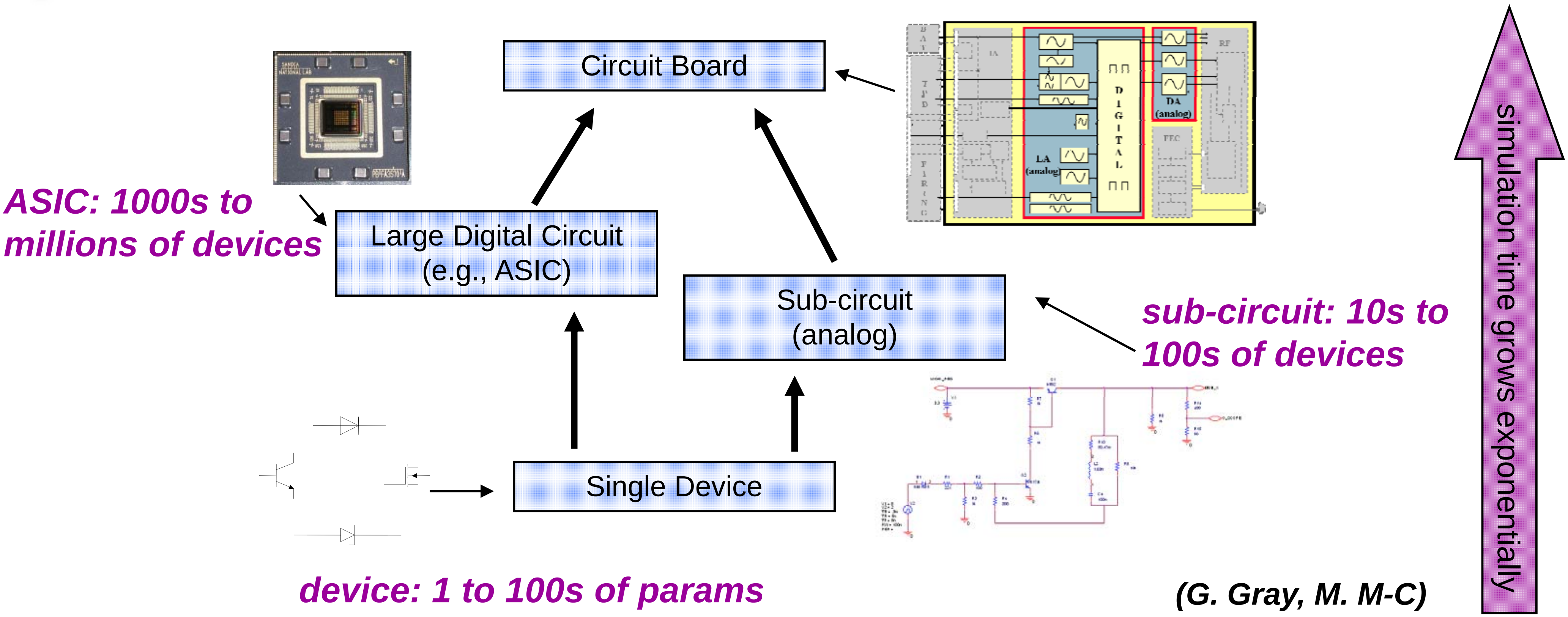


Patty Hough
8964

Laura Swiler
1411

- John Eddy (6342)
- Bill Hart (1412)
- Karen Haskell (9326)
- John Siirola (1433)

Electrical Modeling Complexity



- **simple devices:** **1 parameter, typically physical and measurable**
- **e.g., resistor @ 100Ω +/- 1%**
- **resistors, capacitors, inductors, voltage sources**

- **complex devices:** **many parameters, some physical, others "extracted" (calibrated)**
- **multiple modes of operation**
- **e.g., zener diode: 30 parameters, 3 bias states; many transistor models (forward, reverse, breakdown modes)**

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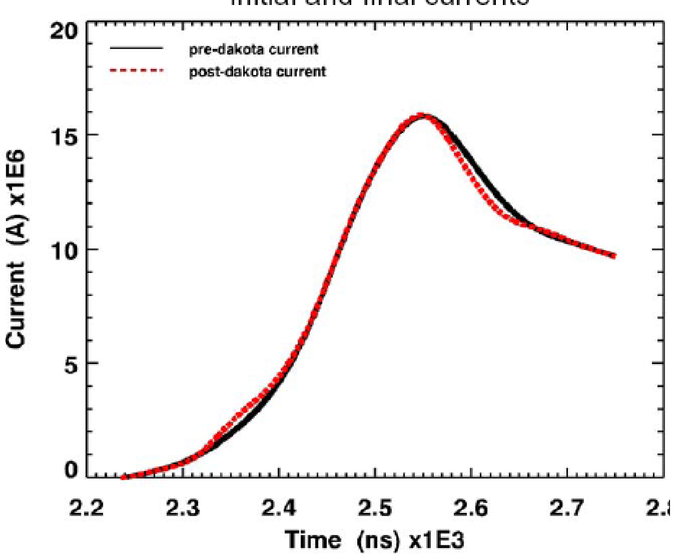
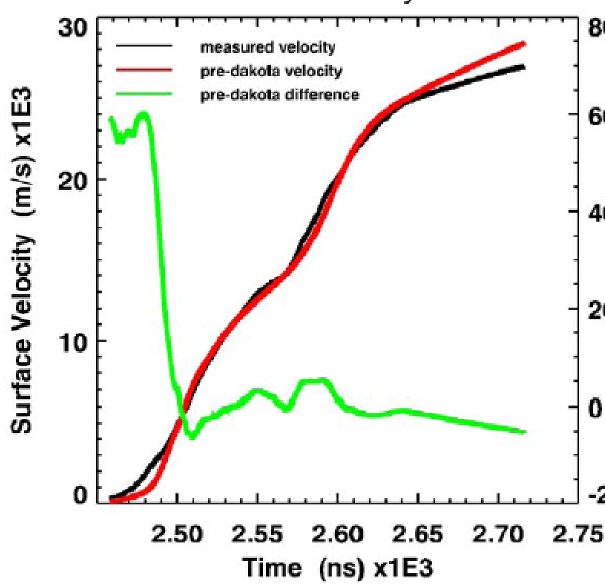
DAKOTA Calibration Study: ALEGRA Simulations vs. Z-Accelerator Data

- **Goal:**
  - Isentropically compress materials and/or shocklessly accelerate flyers to high velocity (~30 km/s) for equation-of-state (EOS) measurements.
  - Increased accuracy in EOS data impacts both NW and inertial confinement fusion applications.
- **Approach:**
  - Current-vs.-time conditions during Z shot not measured with sufficient accuracy for use in ALEGRA simulations.
  - Flyer plate velocity is measured with sufficient accuracy.
  - Solution - DAKOTA optimizes the current waveform (left) to match ALEGRA velocity data to Z velocity data.
- **Results:**
  - Optimized velocity (right) more accurate than initial velocity (center): ***17% vs. 24% max error***
  - The optimized current waveform (left) permits high-fidelity ALEGRA magneto-hydrodynamic simulations.
  - Waveform for shot Z1446 was tuned to eliminate shock formation during compression [shocks preclude getting EOS data].
  - Z1446 post-shot data analysis showed no shock formation in material sample – ***good EOS data***.
  - Future studies: optimize current shapes for Z and ZR shots; uncertainty quantification for Z and ZR shots.
- **Contacts:**
  - DAKOTA - Tony Giunta, Dept. 9133, aagiunt@sandia.gov, 505/844-4280
  - Z & ALEGRA – Ray Lemke, Dept. 1674, rwlemke@sandia.gov, 505/845-7423

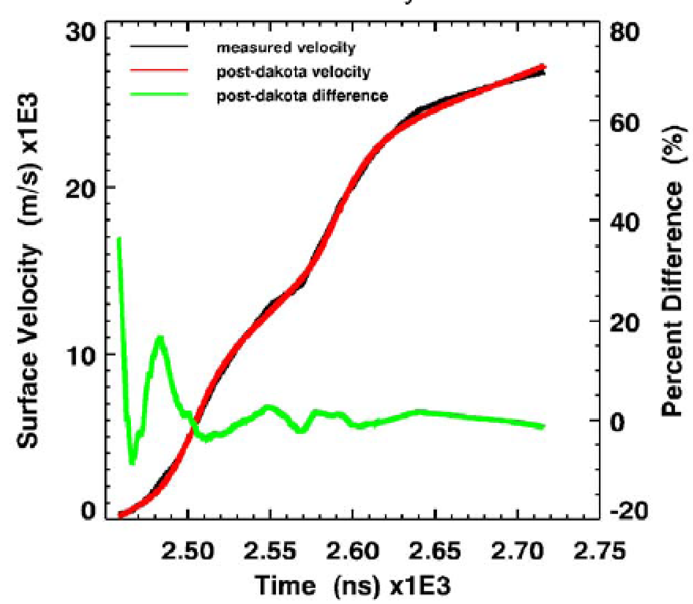
initial and final currents



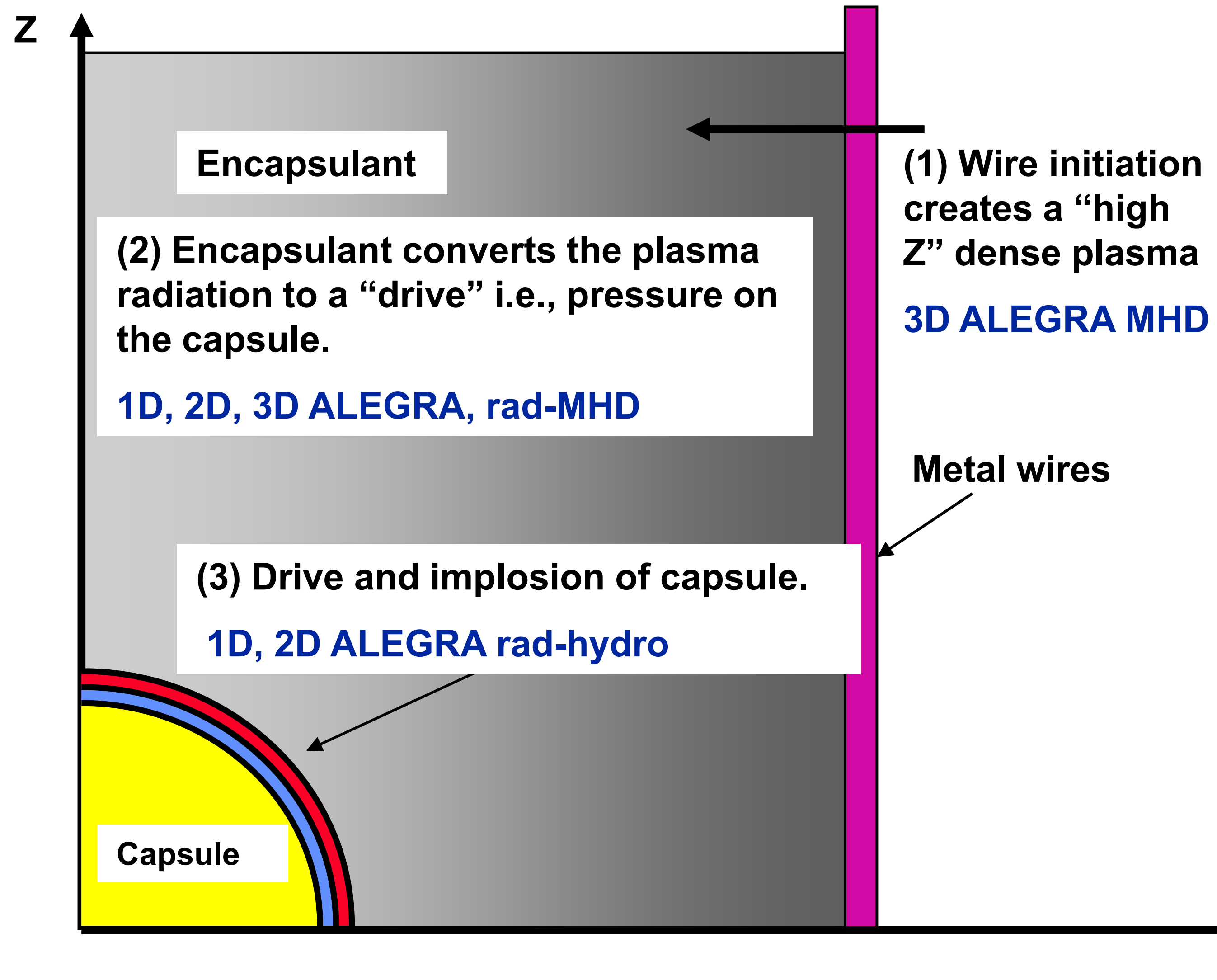
initial and measured flyer velocities

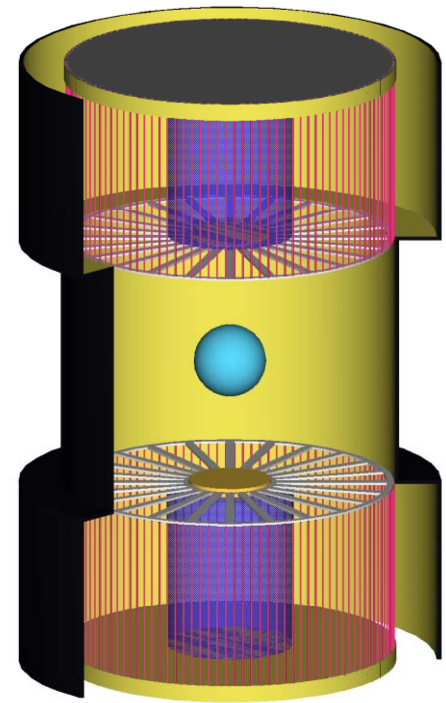


final and measured flyer velocities



Robust Hohlraum Design for Inertial Confinement Fusion



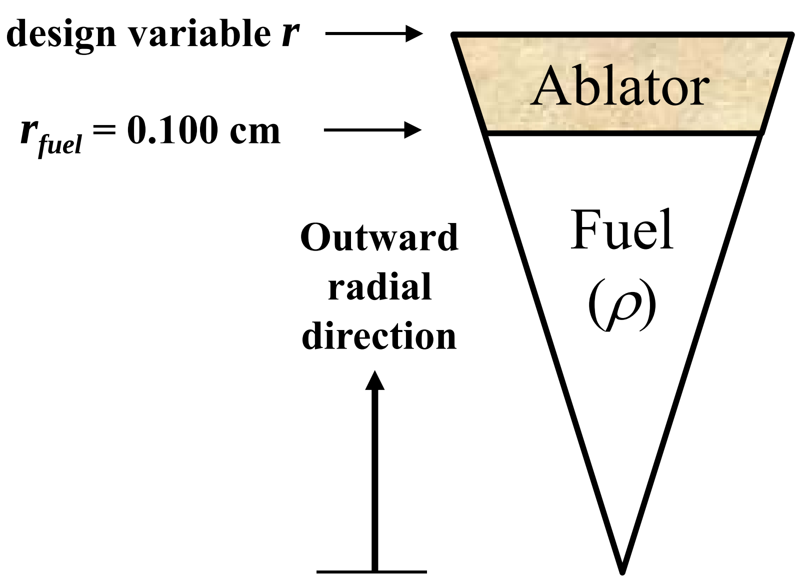


Sample Hohlraum Configuration

Uncertainties in plasma, drive, and capsule characteristics

ICF Capsule Robust Design

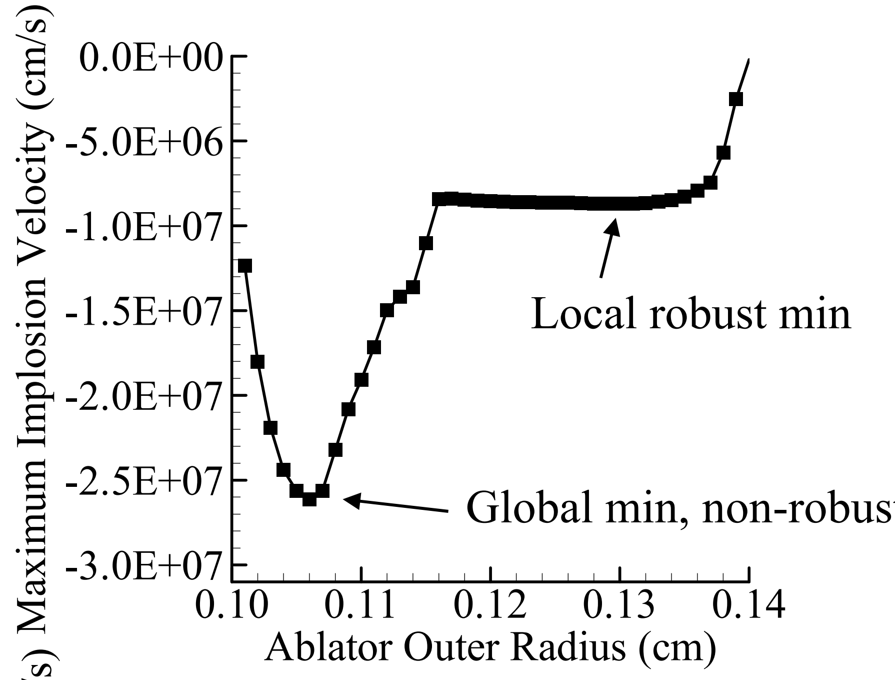
Design goal: maximize the implosion velocity w.r.t. ablator radius *r* and fuel density *ρ*, but remain robust w.r.t. manufacturing variability

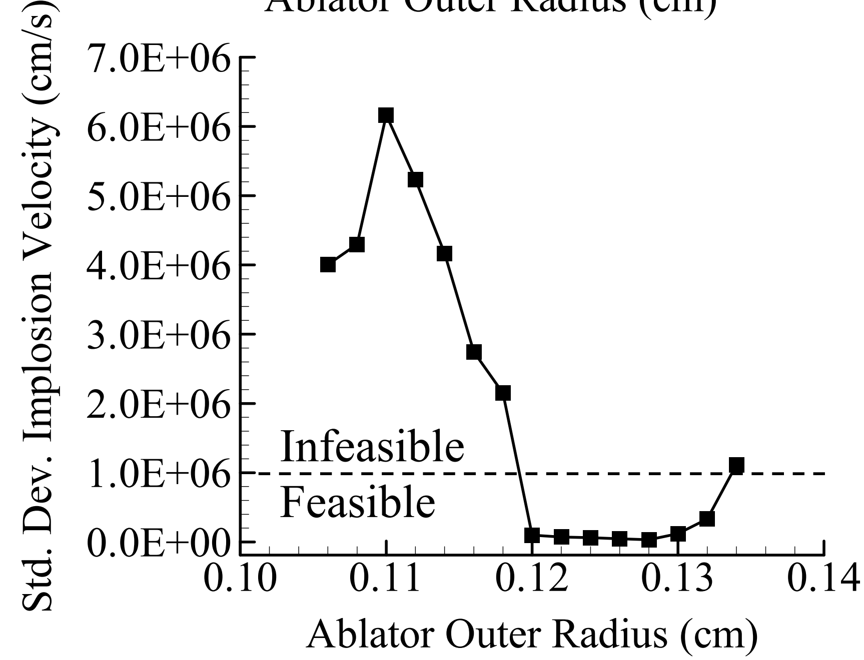


Minimize $V(r, \rho)$

Subject to $\sigma_V(r, \rho) \leq$ target value

uniform: +/- 2.5% range in *r*, *ρ*





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Input File for Parameter Study

```
## DAKOTA INPUT FILE - dakota_rosenbrock_2d.in

strategy
  single_method
    graphics tabular_graphics_data

method
  multidim_parameter_study
  partitions = 8 8

model
  single

variables
  continuous_design = 2

    lower_bounds    -2.0      -2.0
    upper_bounds     2.0       2.0
    descriptors      'x1'      "x2"

interface
  direct
  analysis_driver = 'rosenbrock'

responses
  num_objective_functions = 1
  no_gradients
  no_hessians
```

DAKOTA 5.0 Highlights

- GNU Lesser General Public License (enables library use of DAKOTA)

- All new JAGUAR 2.0 graphical user interface for creating, editing, and running DAKOTA input files (BSD-like license)
- DAKOTA modules on SNL compute clusters (`module avail dakota`)
- Creation and management of evaluation working directories
- Parallelism examples; pre/post run; Mac / Windows binaries

- Additional discrete variable types; supported by parameter studies, nondeterministic sampling (discrete distributions), JEGA, and COLINY
- Stochastic expansion: Anisotropic sparse grids, numerically-generated orthogonal polynomials, and improved expansion tailoring; *many more not detailed here!*
- New epistemic and mixed aleatory-epistemic UQ: local/global interval estimation and local/global evidence.

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Getting Started with DAKOTA

- **Access a Sandia installation (preferred)**
  AMECH (CA), CEE (ESHPC/SCICO, NM), Computer clusters (both)
  or download (Analyst Home Page or DAKOTA webpage)
- **Attend a DAKOTA training class**
- **User's Manual, Chapter 2: Tutorial, corresponding examples distributed with DAKOTA**
- **Support:**
  - **dakota-users@software.sandia.gov**
    (DAKOTA team and internal/external user community)
  - **dakota-developers@development.sandia.gov**
    (for SNL-specific or issues involving proprietary information)

DAKOTA Training Classes

New modular format:

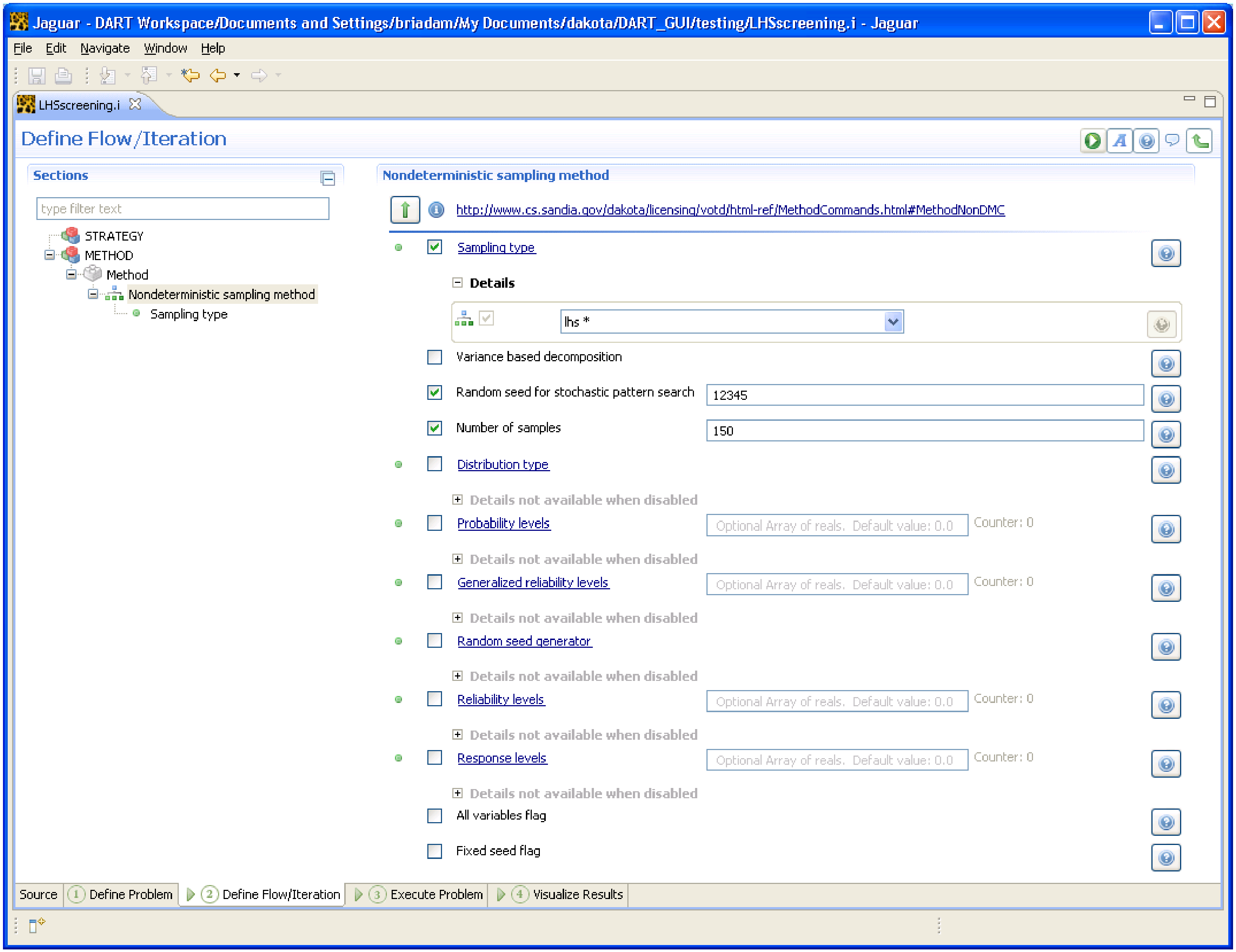
- **DAKOTA 101 (intro to using DAKOTA)**
  half day, interactive lecture, optional hands-on (laptop)

- **Interface DAKOTA to your application**
  half day, hands-on small group workshop

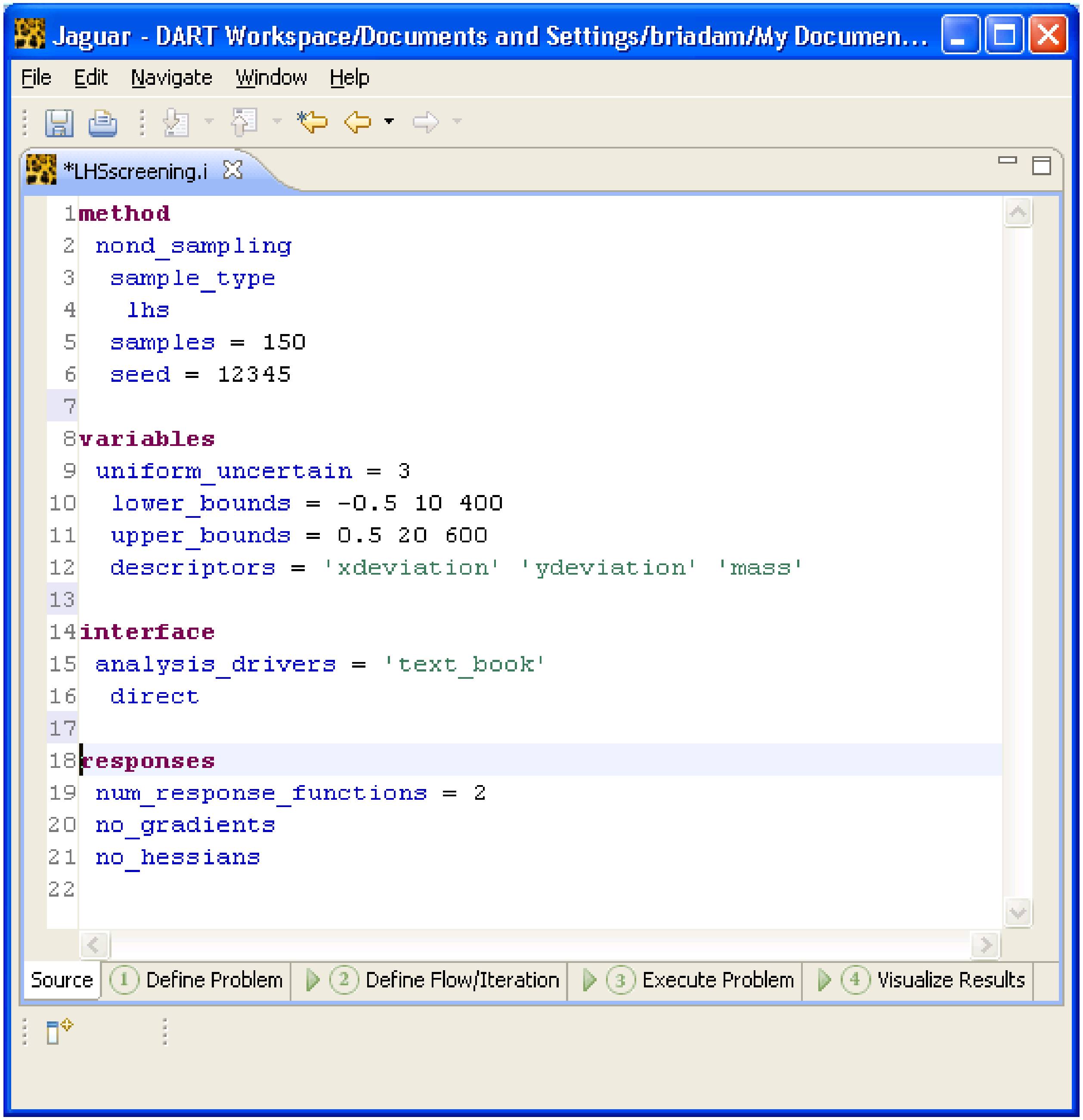
- **Advanced topics in DAKOTA User's Group Meetings**

- **Method theory and selection (2 hours each):**
  - **Sensitivity analysis / screening**
  - **Optimization and calibration**
  - **Uncertainty quantification**

JAGUAR Graphical Editor



JAGUAR Text Editor



JAGUAR Sensitivity Analysis Wizard