DAKOTA 4.2 Overview

"What is DAKOTA and how might your work benefit from it?"

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DAKOTA Product Manager

Optimization and Uncertainty Quantification (1411)

Unlimited Release: SAND 2008-7901 P

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

DAKOTA Overview Goals

A very basic introduction to DAKOTA and its methods

- **Through application examples and a method introduction, help you decide if DAKOTA might be relevant for your work**

- **For current users: briefly survey new features in DAKOTA 4.2**

DAKOTA in a Nutshell

Design and Analysis toolKit for Optimization and Terascale Applications

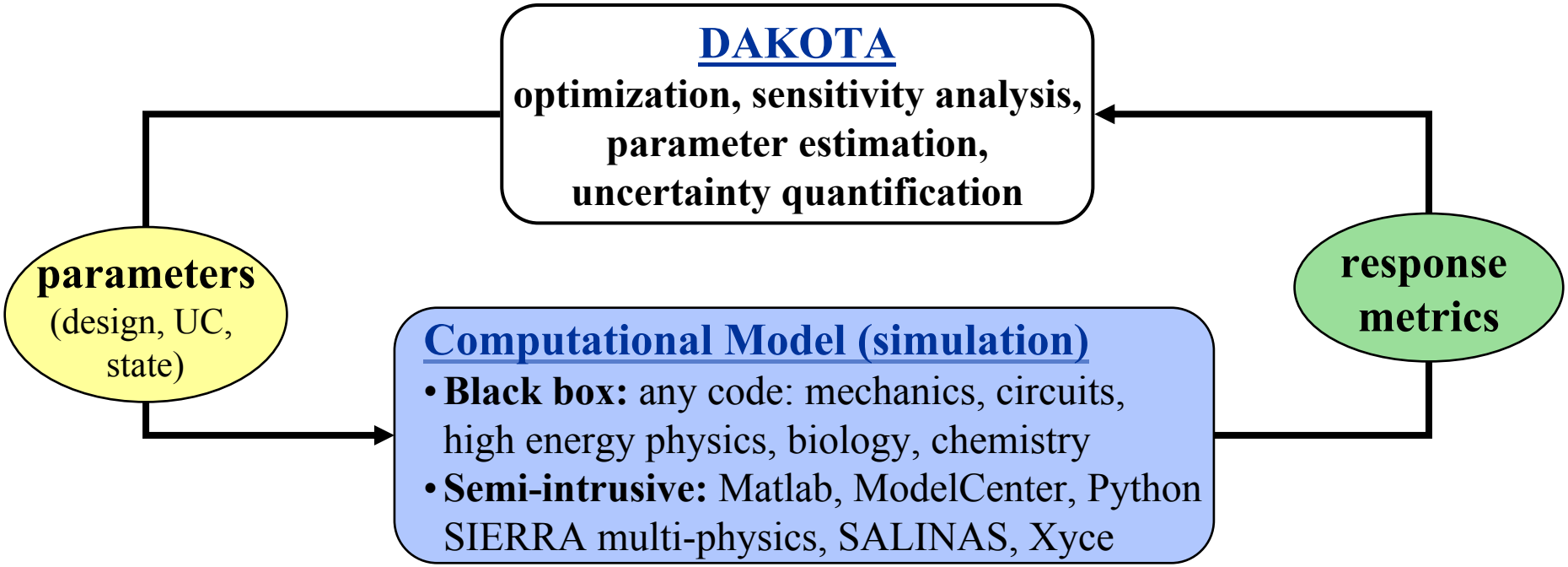
Answer fundamental science and engineering questions with computational models (simulations)

- **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 (examples of each upcoming)***

Automated Iterative Analysis

Automate typical "parameter variation" studies with a generic interface 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 simulations that are: nonsmooth, discontinuous, multimodal, expensive, mixed variable, failure-prone
- Supports scalable parallel computations on clusters
- Strategies to combine methods for advanced studies or improve efficiency with surrogates (meta-models)
- Object-oriented code; modern software quality practices
- Limited Windows interface (run via command prompt); graphical user interface and DART integration in progress

- Additional details: http://www.cs.sandia.gov/dakota
  - Extensive documentation, including a tutorial
  - Support mailing lists
  - Software downloads: stable releases and nightly builds (freely available worldwide via GNU GPL)

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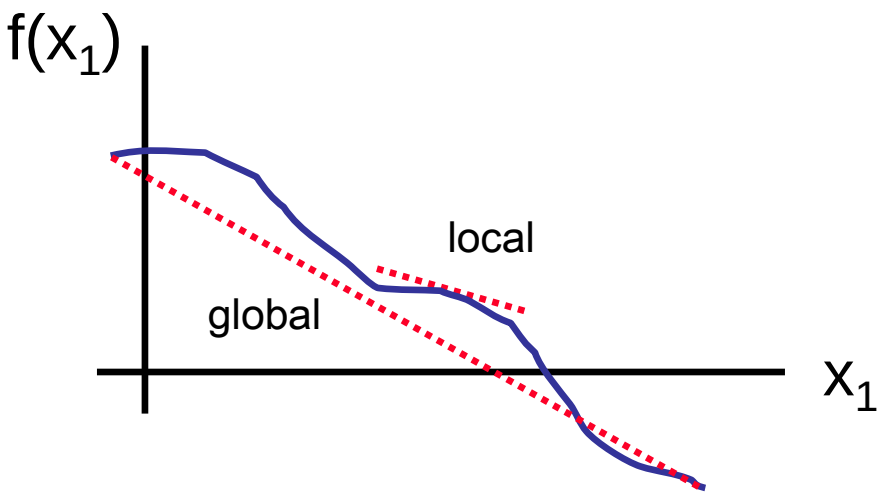
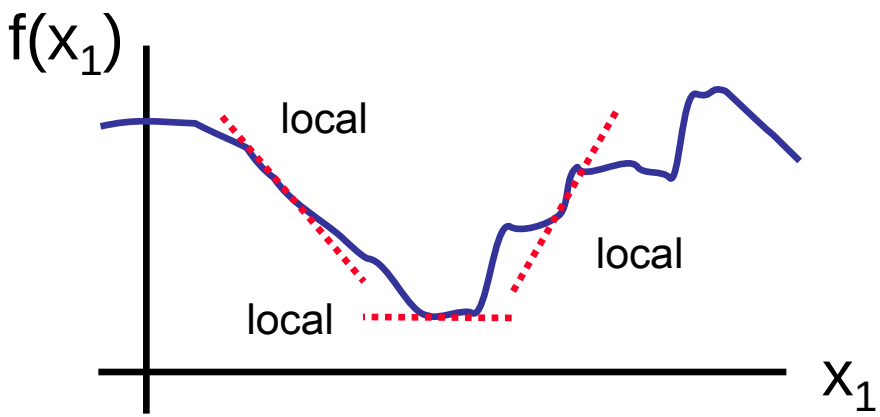
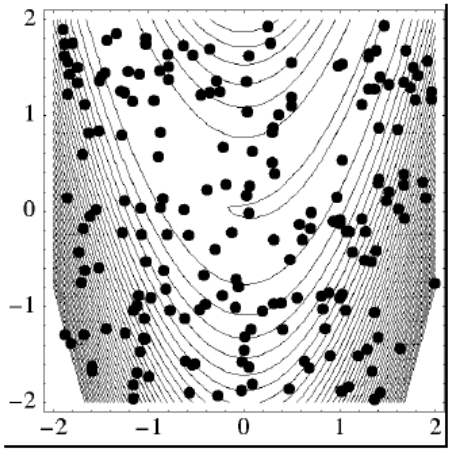
Sensitivity Analysis

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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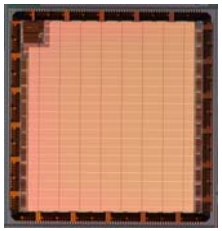
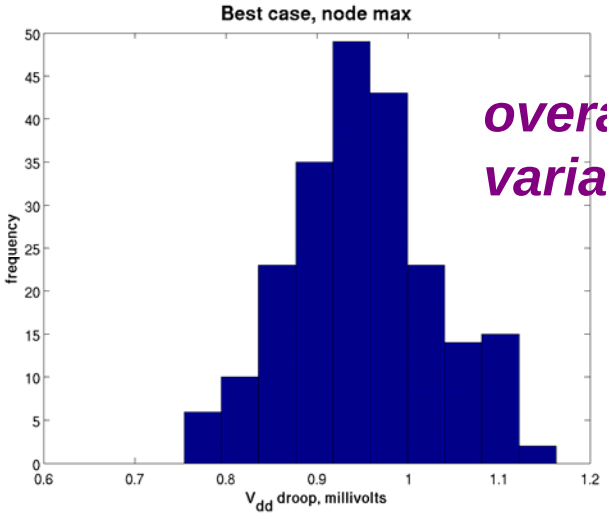
SA for Electrical Circuits

- **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)



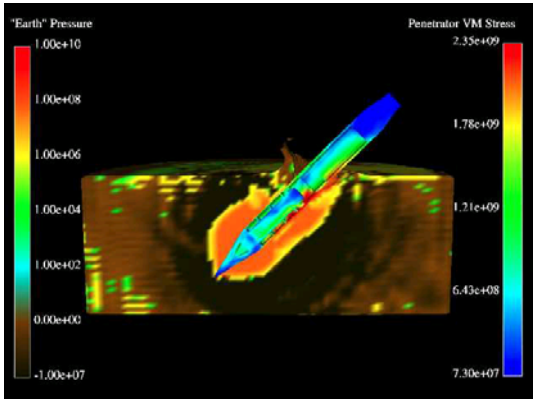
	Vdd Metrics	
	node max	node avg
METAL1	0.96	0.82
METAL2	0.11	0.04
METAL3	0.10	0.05
METAL4	0.80	0.81
METAL5	0.86	0.91
VIA1	0.71	0.66
VIA2	0.80	0.76
VIA3	0.57	0.60
VIA4	0.91	0.94
CONTACT	0.21	0.13
polyc	0.04	0.05

correlations

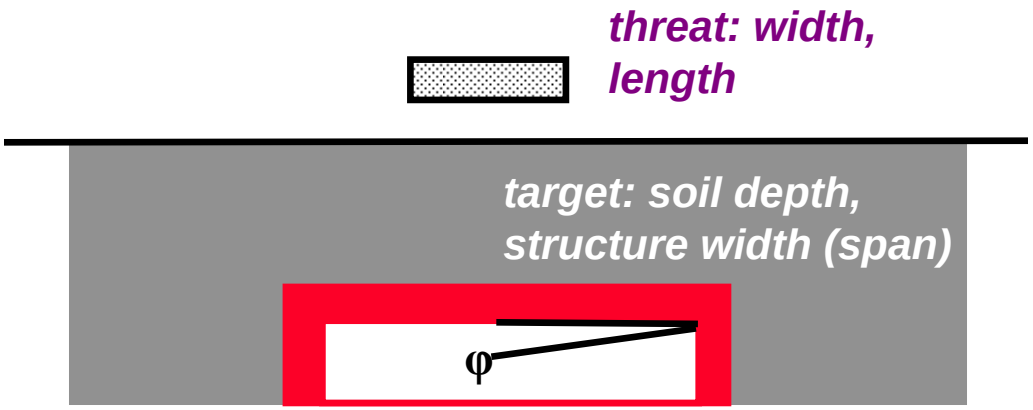


overall variability

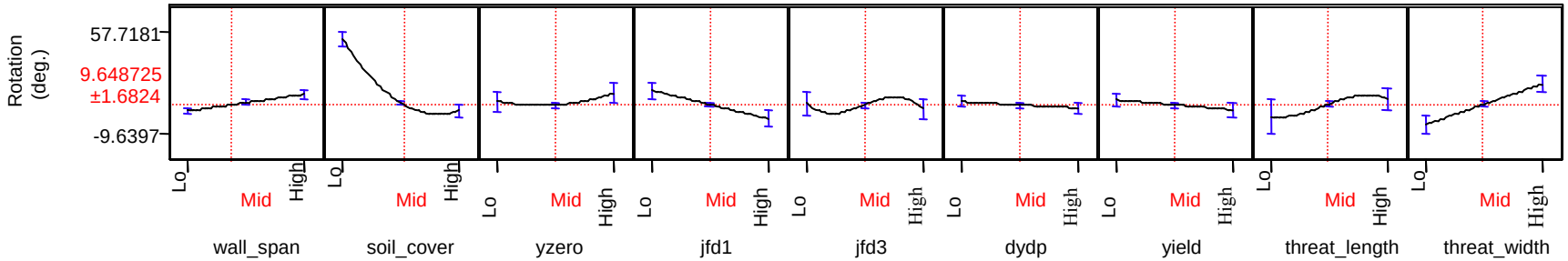
SA of Penetrator



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

- DAKOTA includes 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)
  - Monte Carlo, Latin hypercube sampling (with correlation or variance analysis, including variance-based decomposition)
  - Mean-value with importance factors

- DAKOTA outputs basic statistics on responses, including mean, standard deviation, and correlations; DAKOTA tabular output typically analyzed with third-party statistics package
- In addition to main effects, can determine 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

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

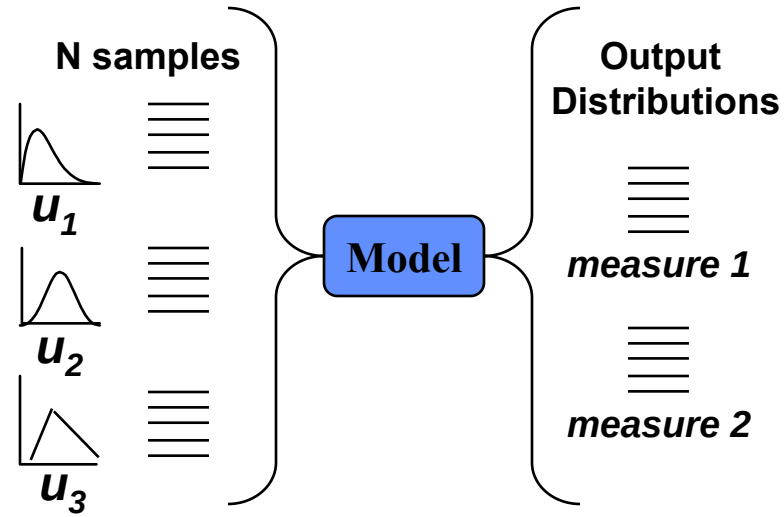
→ **Computational Model** →

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

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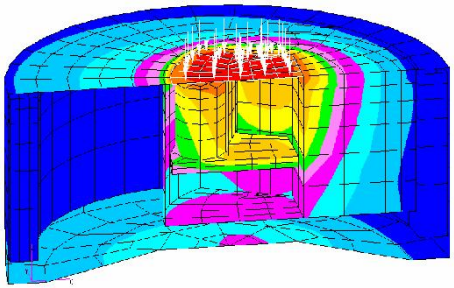
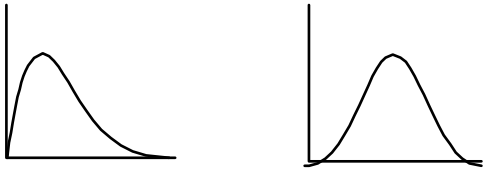
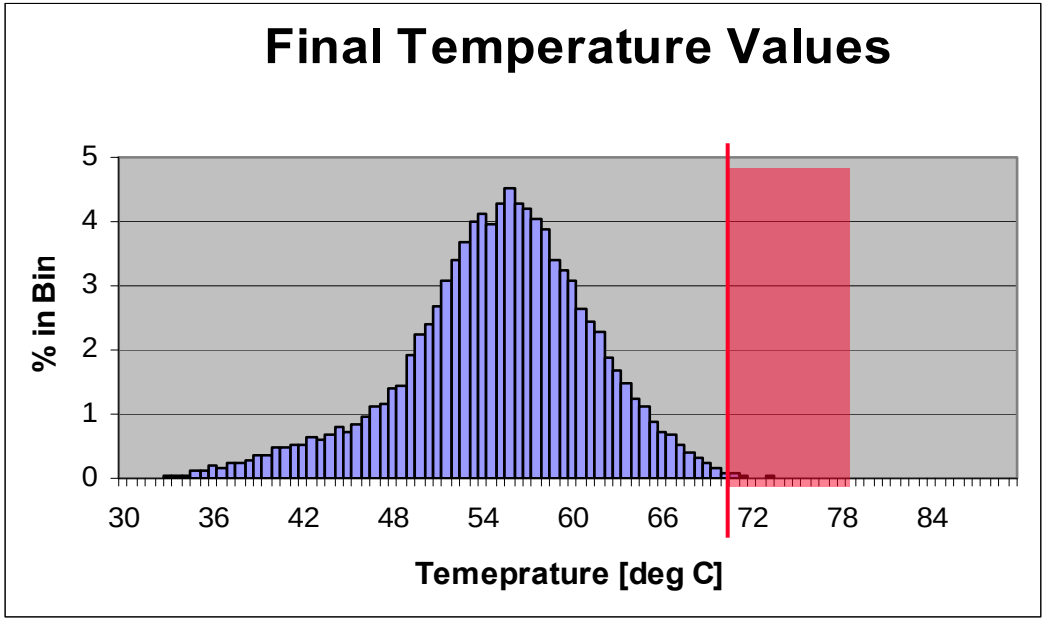
Uncertainty Quantification

- **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:

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

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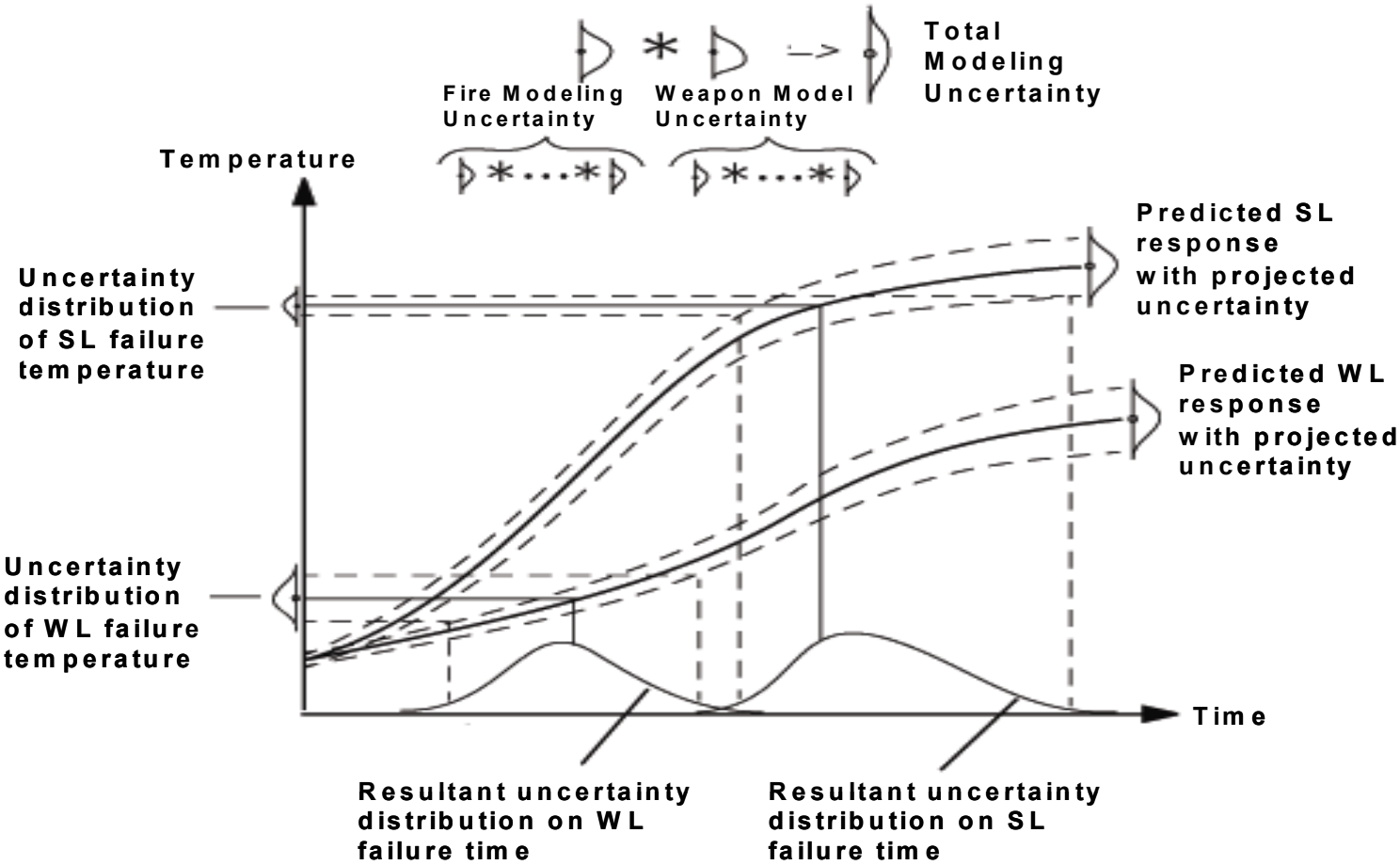
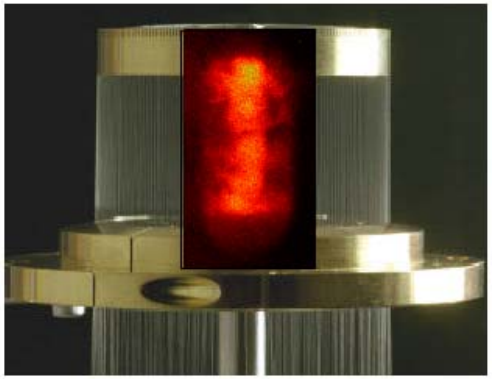
UQ for Thermal Race

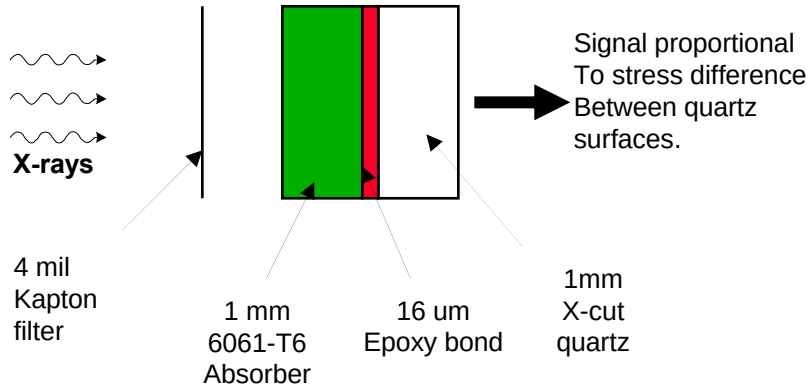


UQ for Validation: Presto Simulations vs. Z-Accelerator Data

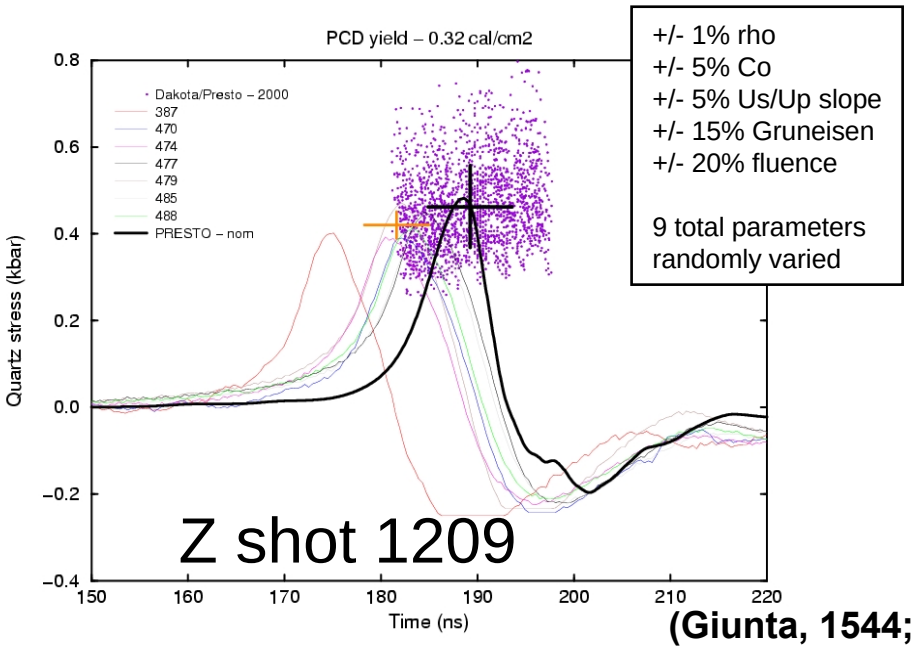
Tungsten wire array & Z pinch

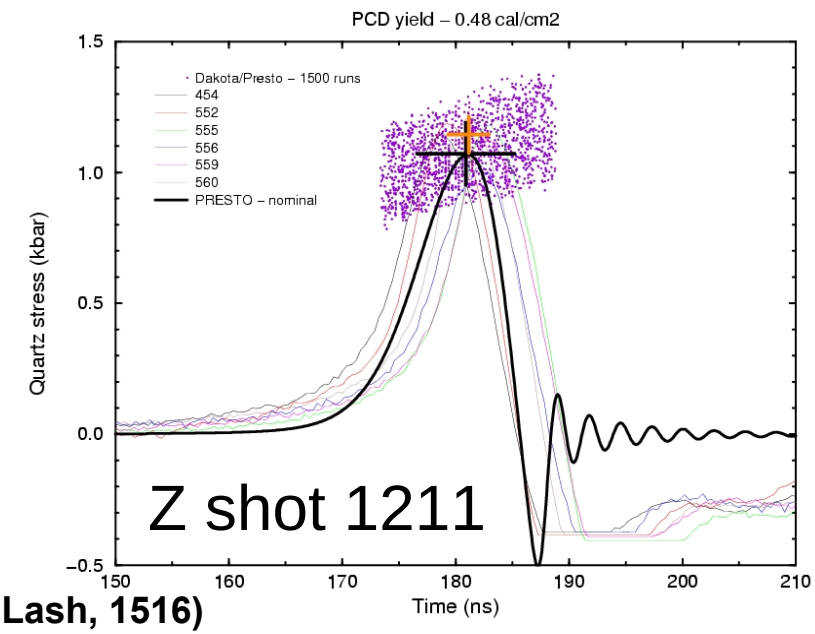


X-Ray Induced Thermomechanical Shock Modeled w/ Presto



- **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**





(Giunta, 1544; Lash, 1516)

DAKOTA UQ

- DAKOTA techniques for propagating uncertainty through models:
  - Latin hypercube sampling (and other sampling approaches)
  - Local reliability methods (mean value, MPP search, FORM)
  - Global reliability methods (EGRA)
  - Non-intrusive stochastic expansion methods (polynomial chaos and stochastic collocation)
  - Dempster-Shafer evidence theory (belief/plausibility)

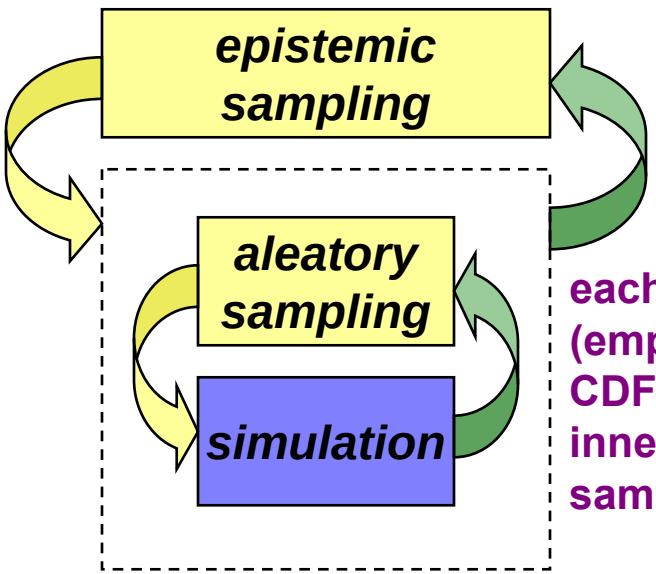
- DAKOTA can output probability of response thresholds, reliability metrics, response corresponding to a metric, etc.

- In addition to aleatory uncertainty (variables characterized by probability distributions), DAKOTA permits studies with epistemic uncertainty (variables characterized by intervals or basic probability assignments).

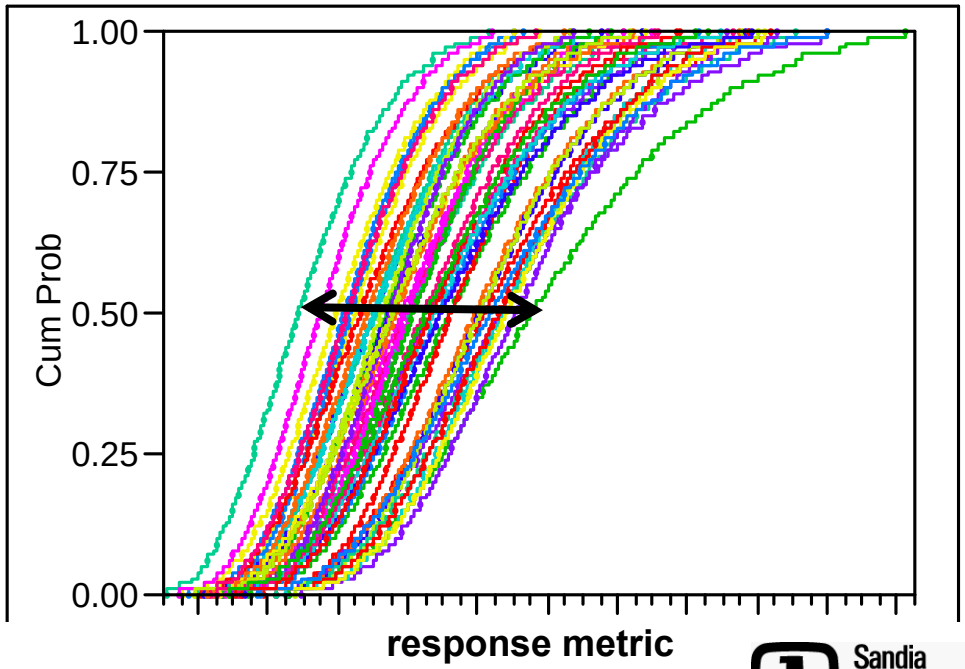
"Second-Order" Probability

- **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



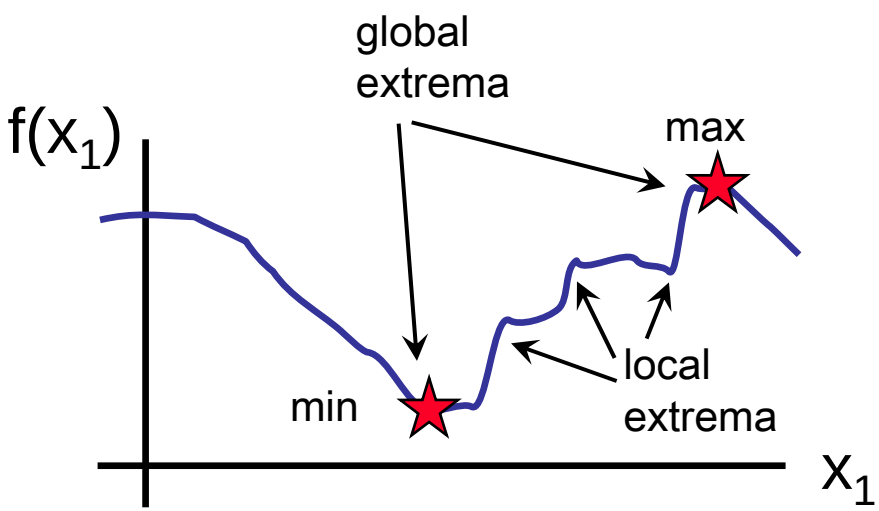
each discrete (empirical) CDF: 100 inner loop samples



"Envelope" of CDF traces represents response epistemic uncertainty

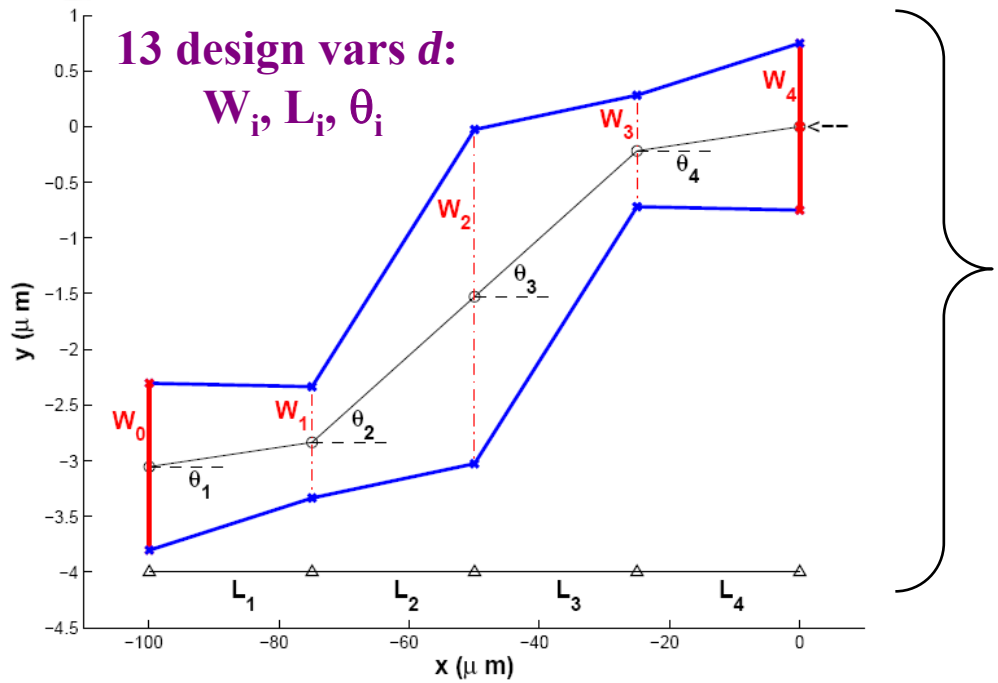
Optimization

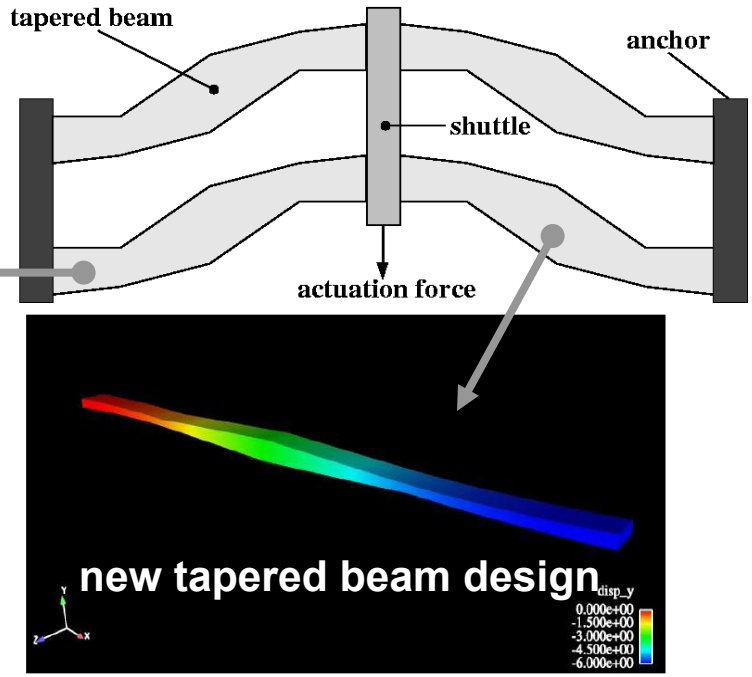
- **GOAL: Vary parameters to extremize objectives, while satisfying constraints to find (or tune) the best design, estimate best parameters, analyze worst-case surety, e.g., determine:**
  - **delivery network that maximizes profit while minimizing environmental impact**
  - **case geometry that minimizes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

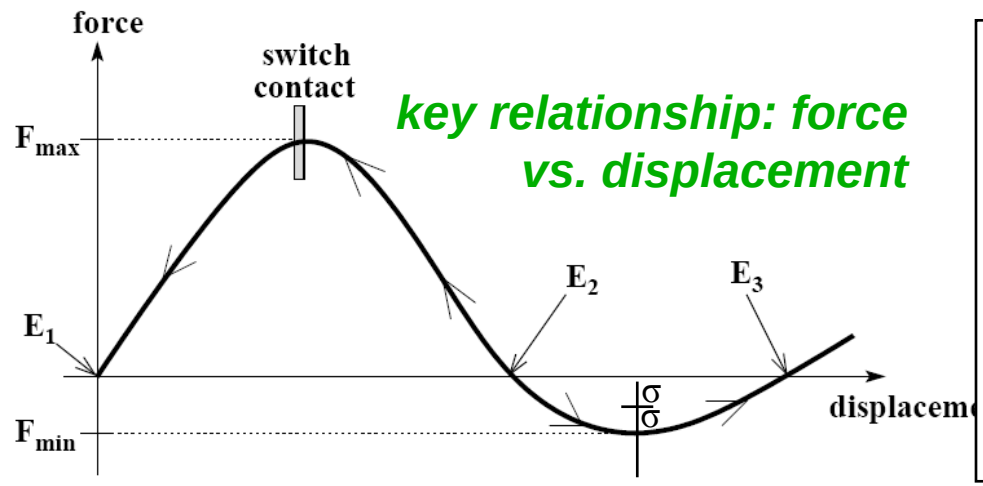


Some applications: local improvement suffices; others: must find global minimum at any cost

MEMS Switch Design: Geometry Optimization





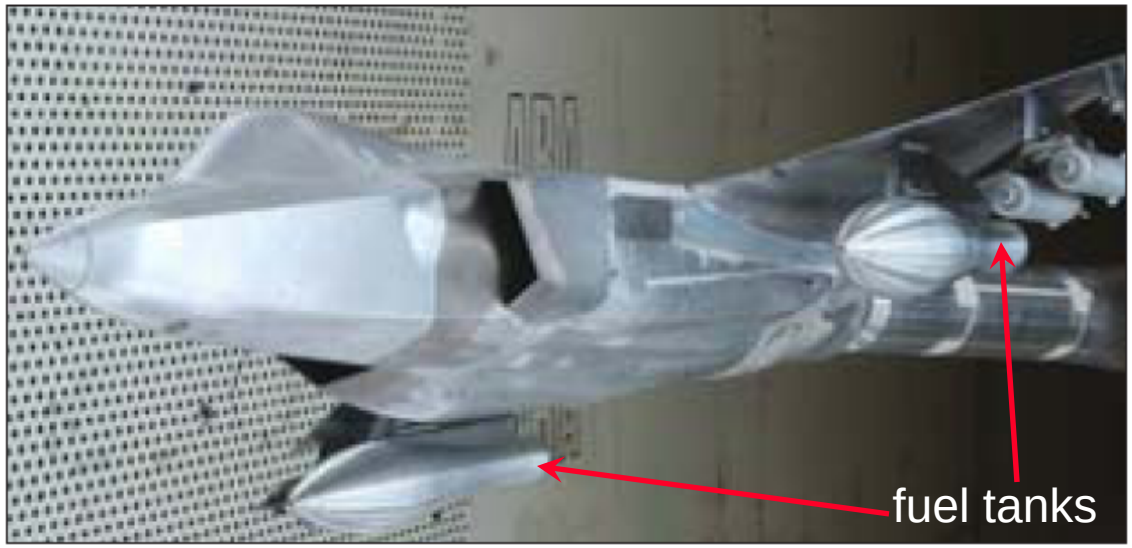


key relationship: force vs. displacement

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)

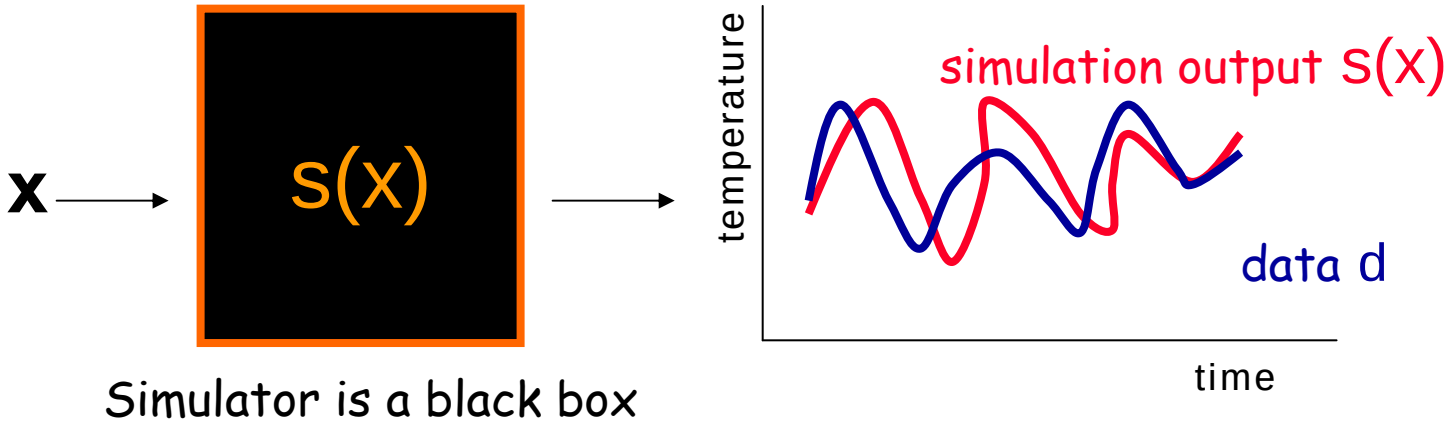
Derivative-free methods

- 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)*

Calibration/Parameter Estimation

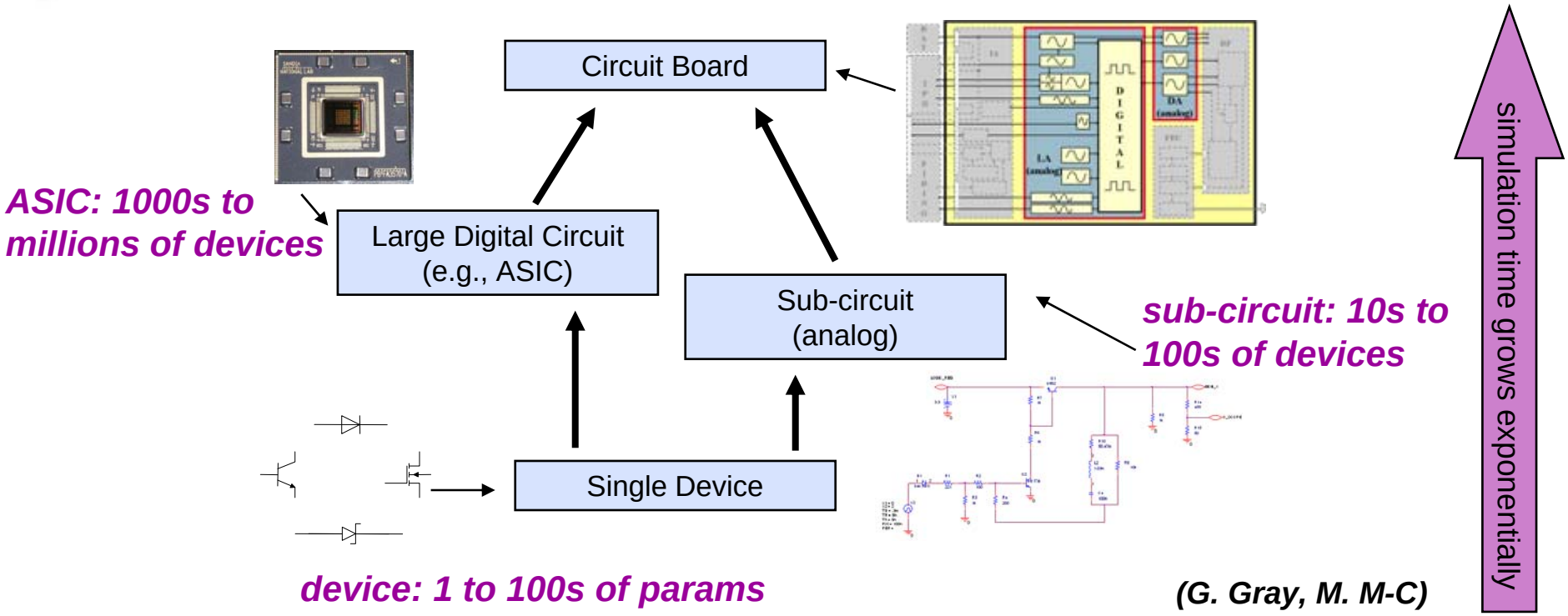
$$f(x) = \sum_{i=1}^{n} (\underbrace{s_i(x)}_{\text{Simulation output that depends on } x} - \underbrace{d_i}_{\text{Given data}})^2$$



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)

Electrical Modeling Complexity

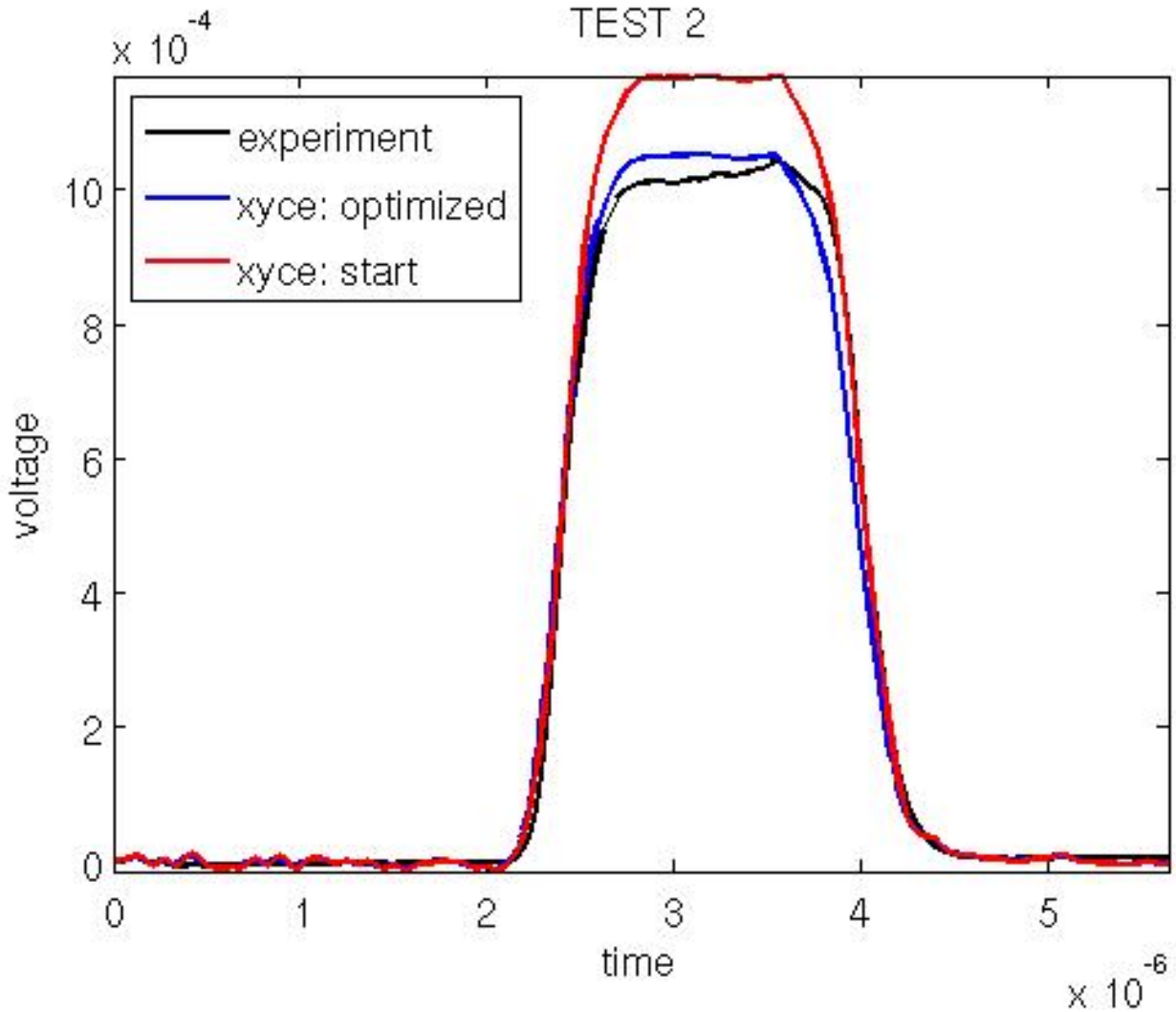


- **simple devices:** 1 parameter, typically physical and measurable
- e.g., resistor @ 100Ω +/- 1%
- resistors, capacitors, inductors, voltage sources

- **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)

Sample Signal Calibration

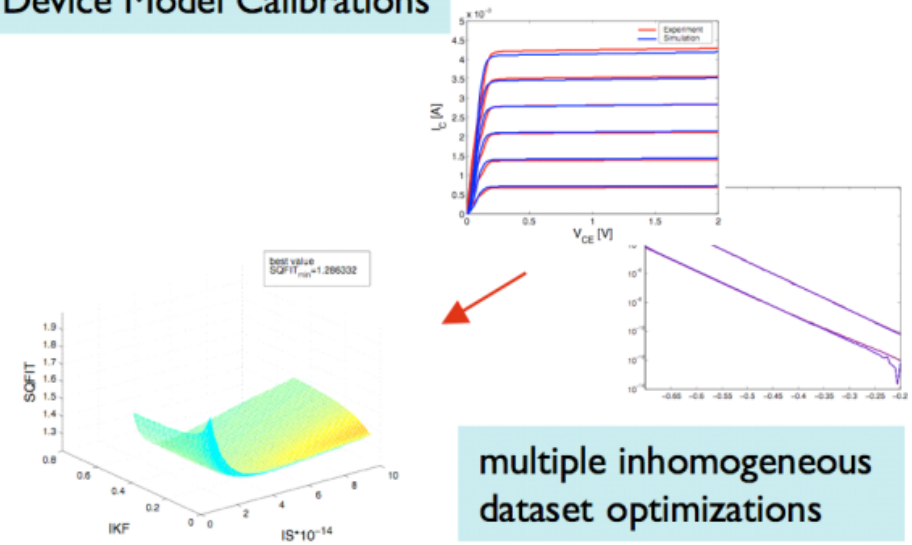
- **Calibration of 8 circuit parameters to match experimental signal (G. Gray, M. M-C)**



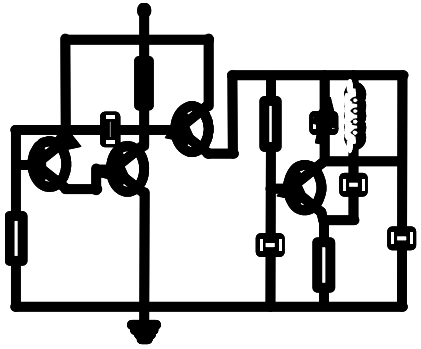
QASPR Model Calibration

- **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

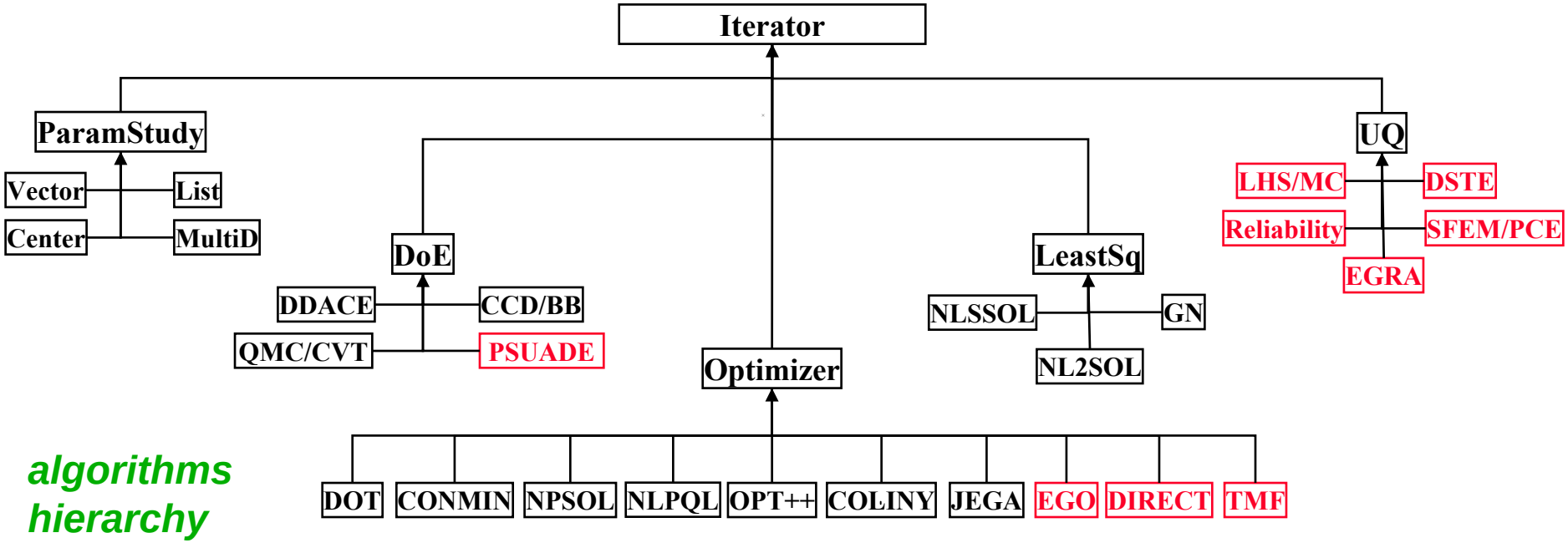


multiple inhomogeneous dataset optimizations



Summary: DAKOTA Framework

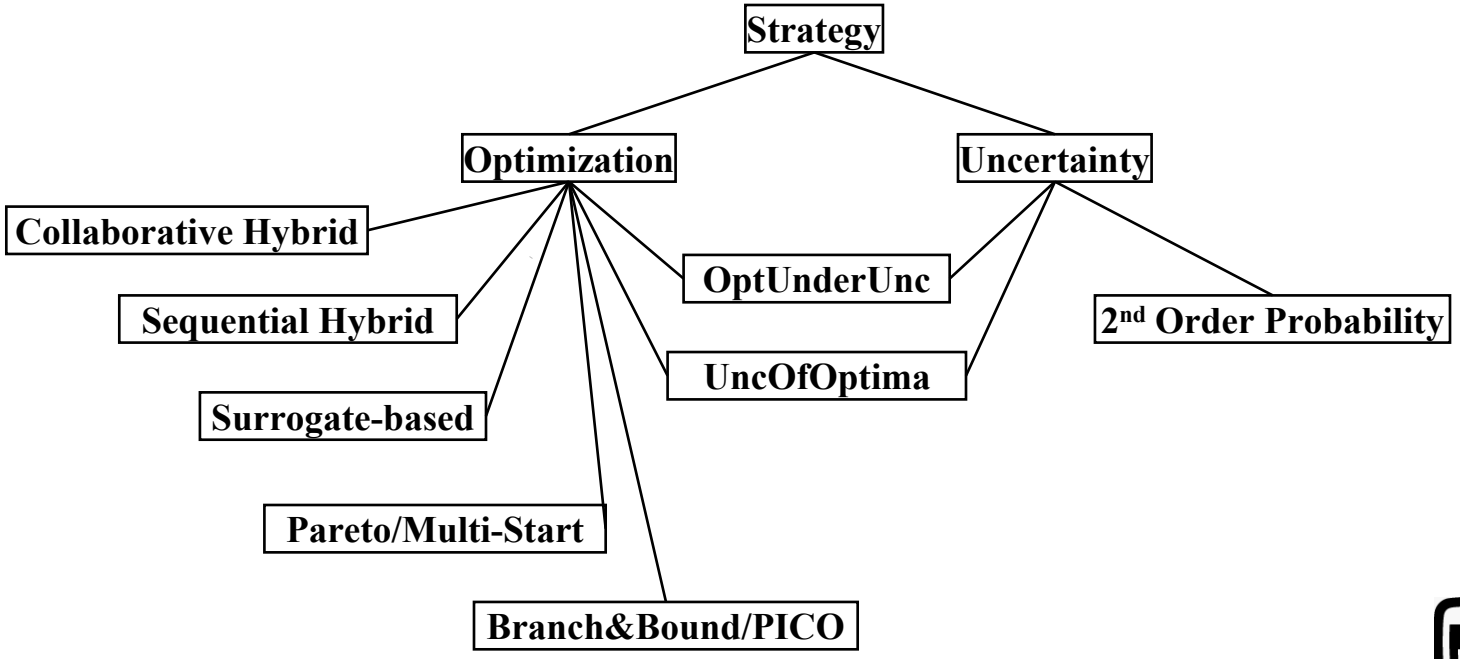
Unified software infrastructure: **reuse tools and common interfaces;** ***integrate commercial, open-source, and research algorithms***



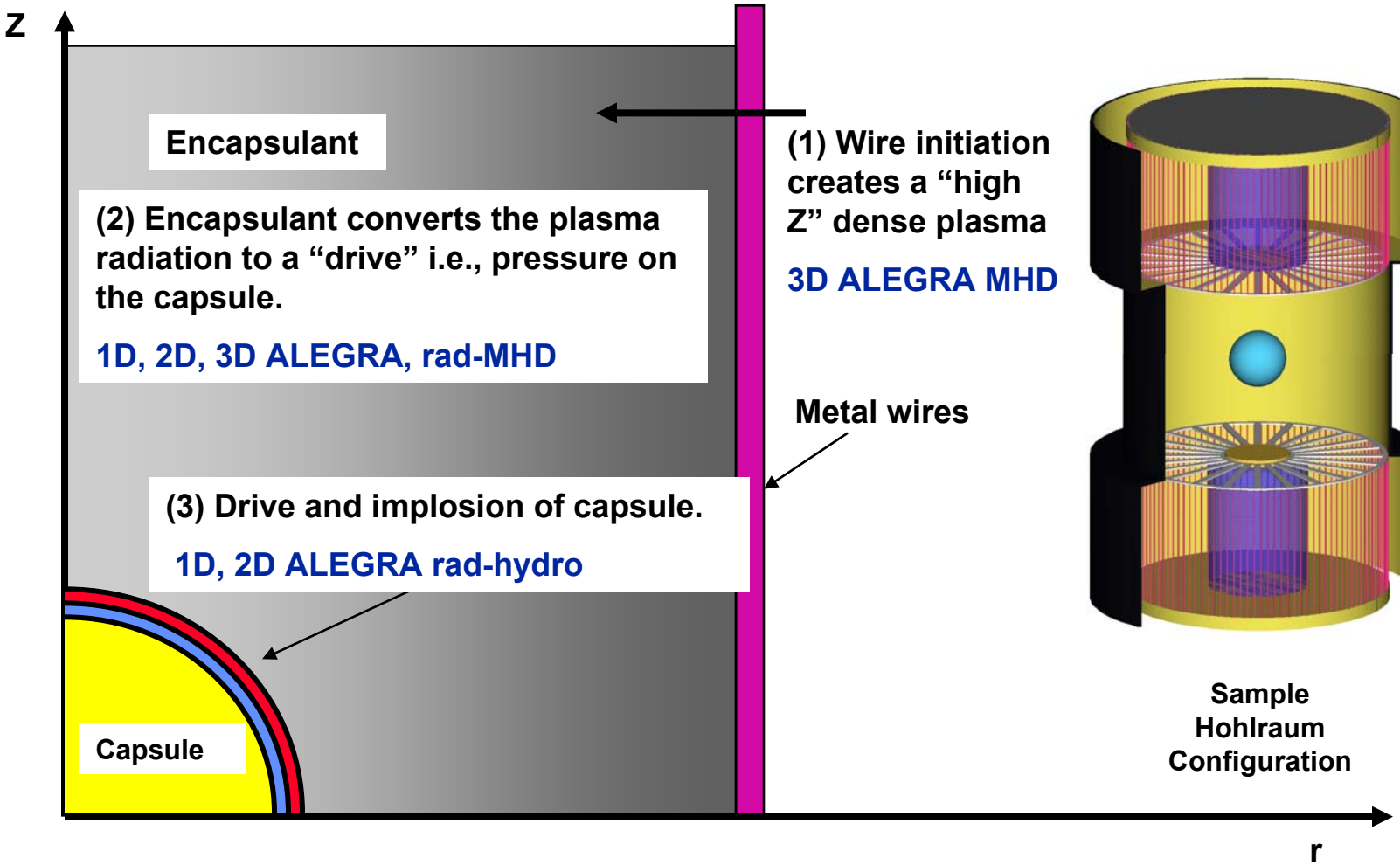
algorithms hierarchy

Advanced Features

- DAKOTA strategies enable flexible combination of multiple models and algorithms
  - Nested, layered, cascaded, concurrent, adaptive, interactive
  - Optimization under uncertainty, reliable/robust design
  - Surrogate-based optimization
  - Calibration of simulation moments to data



Robust Hohlraum Design for Inertial Confinement Fusion



Sample Hohlraum Configuration

Uncertainties in plasma, drive, and capsule characteristics

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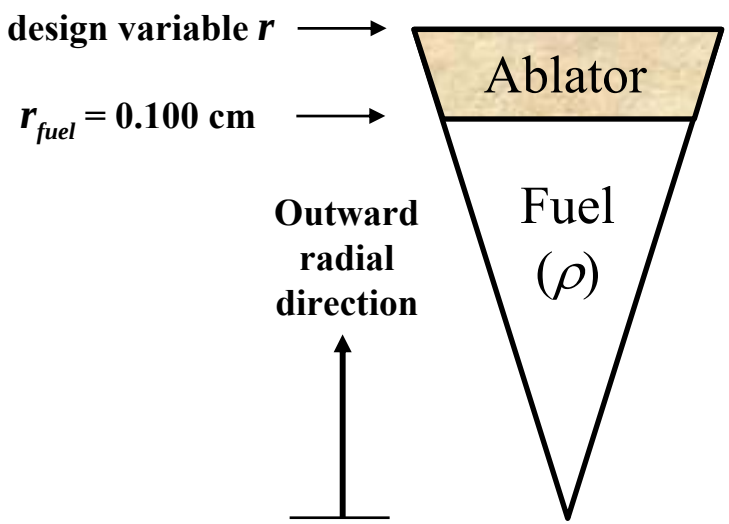
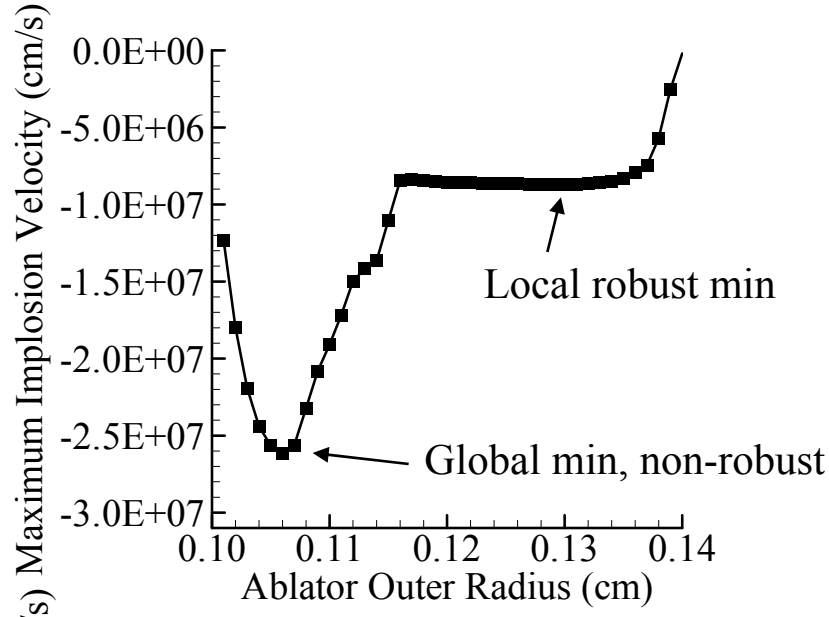
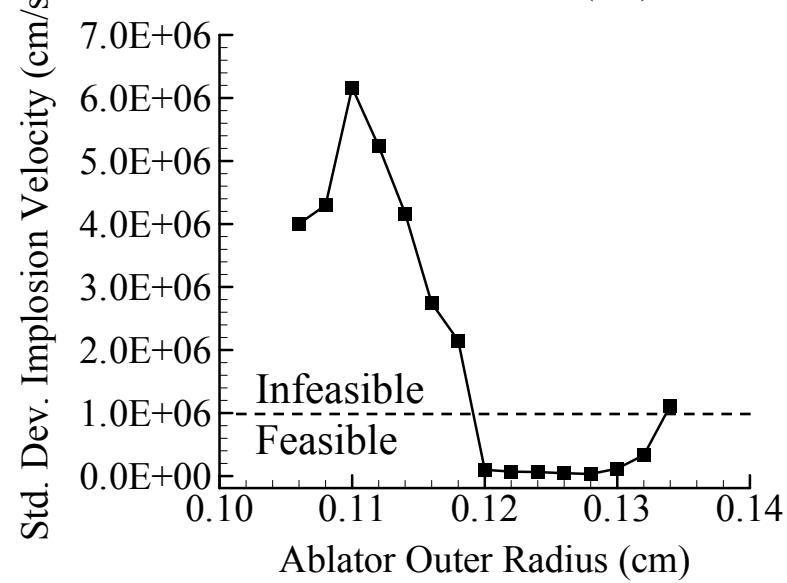
ICF Capsule Robust Design

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

New Capability in DAKOTA 4.2

- **Uncertainty quantification**
  - **stochastic collocation method via Lagrange polynomial interpolation**
  - **more scalable and higher order generalized polynomial chaos (and SC) methods** *(Smolyak sparse grids w/ mixed integration rules and numerically generated polynomials)*
  - **extended Latin hypercube sampling distributions (Gumbel, Frechet), variable transformations, incremental random sampling**

- **Optimization and calibration**
  - **new bi-level, sequential, and multifidelity optimization under uncertainty algorithms based on stochastic collocation and polynomial chaos**
  - **new APPSPACK interface to directly handle linear/nonlinear constraints**
  - **generalization of efficient global optimization technique**
  - **new capability for surrogate-based model calibration**
  - **improved support for model calibration under uncertainty and weighted nonlinear least squares**

New Capability in DAKOTA 4.2

- **Framework**
  - new radial basis function and moving least squares surrogates
  - more efficient evaluation cache
  - model recursion refinements
  - improved analysis driver specification

- **Usability**
  - newly designed input parser with better feedback on errors
  - additional method tutorials and examples demonstrating coupling DAKOTA to parallel simulation codes for analysis
  - improved platform support for Macintosh and Windows
  - more convenient and robust integration into other software libraries, such as Trilinos and Xyce, with special emphasis on efficiency for large-scale applications

Getting Started with DAKOTA

- Access an installation or download the software (see Analyst Home Page or DAKOTA webpage)
- Take a hands-on, day-long DAKOTA training class
- Users Manual, Chapter 2: Tutorial
- We are available to help you get started: dakota-users@software.sandia.gov (includes DAKOTA development team and internal/external user community)

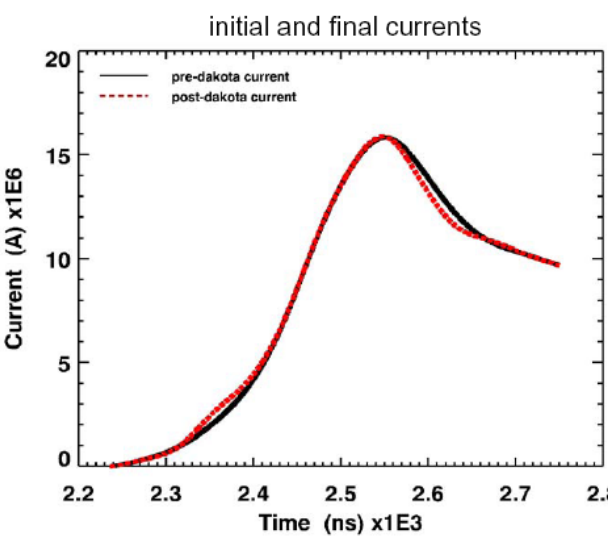
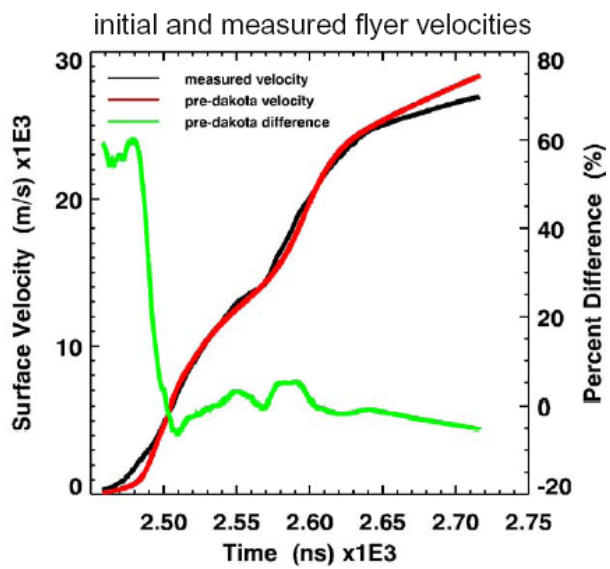
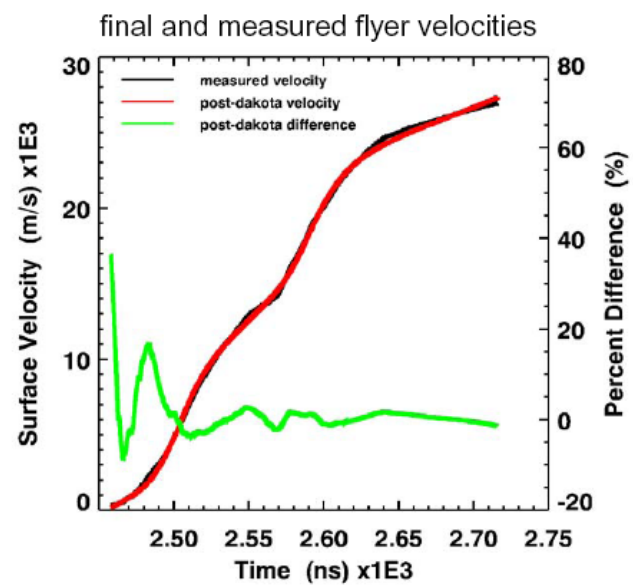
Thank you for your attention!

`briadam@sandia.gov`

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

Sandia National Laboratories

Bonus Slides

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.
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