SAND2015-6794 TR

Dakota Software Training

Dakota Overview

http://dakota.sandia.gov

Sandia National Laboratories

Exceptional service in the national interest

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Module Learning Goals

- What is Dakota?
- Why use Dakota?
- Prerequisites for Using Dakota
- Training outline

WHAT IS DAKOTA?

Dakota enhances simulations…

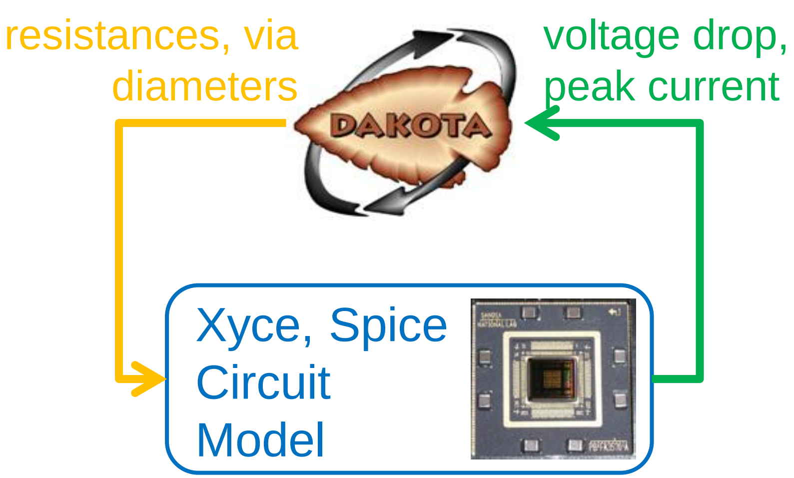
Algorithms for design exploration and simulation credibility

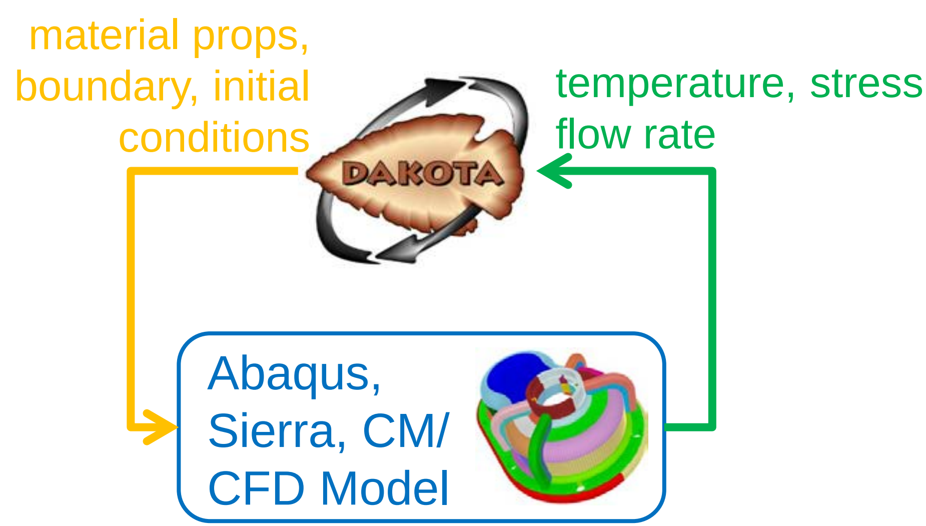
- Suite of iterative mathematical and statistical methods that interface to computational models
- Makes sophisticated parametric exploration of simulations practical for a computational design-analyze-test cycle
- Provides scientists and engineers (analysts, designers, decision makers) greater perspective on model predictions:
  - *Enhances understanding of risk by quantifying margins/uncertainties*
  - *Improves products through simulation-based design, calibration*
  - *Assesses simulation credibility through verification and validation*

…by analyzing ensembles

- Strategically selects model parameters
- Manages concurrent simulations
- Analyzes responses (model outputs)
- ➢ Automates one-pass parameter variation/ analysis to advanced goal-oriented studies

Run	Input	Output
1	0.814	91.3
2	0.906	63.24
…		
N	1.270	9.75





Key Questions Answered

Dakota makes iterative parametric analysis practical for black-box simulations to answer questions of:

- Sensitivity: Which are the crucial factors/parameters?
- Uncertainty: How safe, reliable, or robust is my system?
- Optimization: What is the best performing design or control?
- Calibration: What models and parameters best match data?

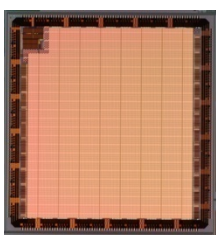
Indirectly:

- Verification: Is the model implemented correctly, converging as expected?
- Validation: How does the model compare to experimental data, including uncertainties?

Enables quantification of margins and uncertainty (QMU) and design with simulations; analogous to experiment-based QMU and physical design/test.

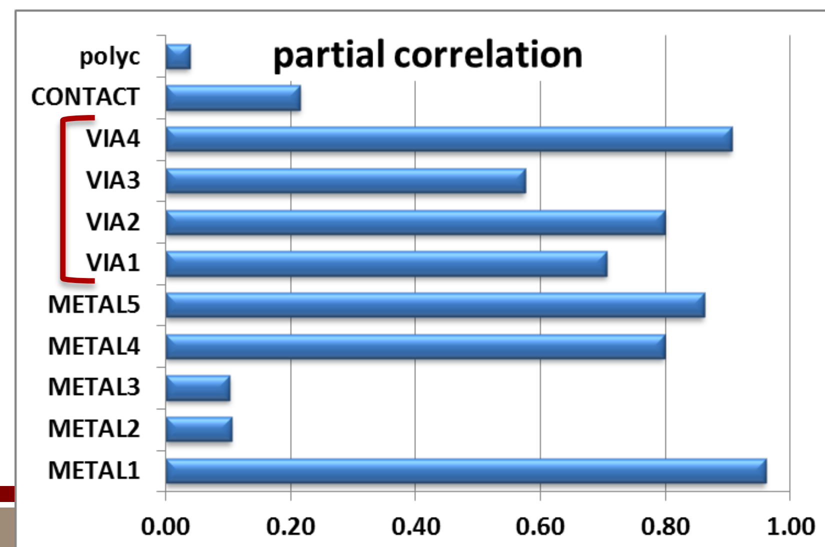
Sensitivity Analysis

- ***Which are the most influential parameters?***
- Interrogate model to assess input/output mapping
  - Expose model characteristics, trends, robustness
  - Focus resources for data gathering or model/code development
  - Screening: reduce variables for UQ or optimization analysis
- Dakota automates common single parameter variations, and provides richer global sensitivity methods



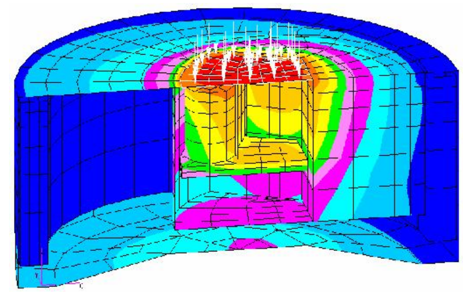
Xyce™ Parallel Electronic Simulator

- Xyce model of CMOS7 ViArray
- Assess influence of manufacturing variability on supply voltage performance during photocurrent event

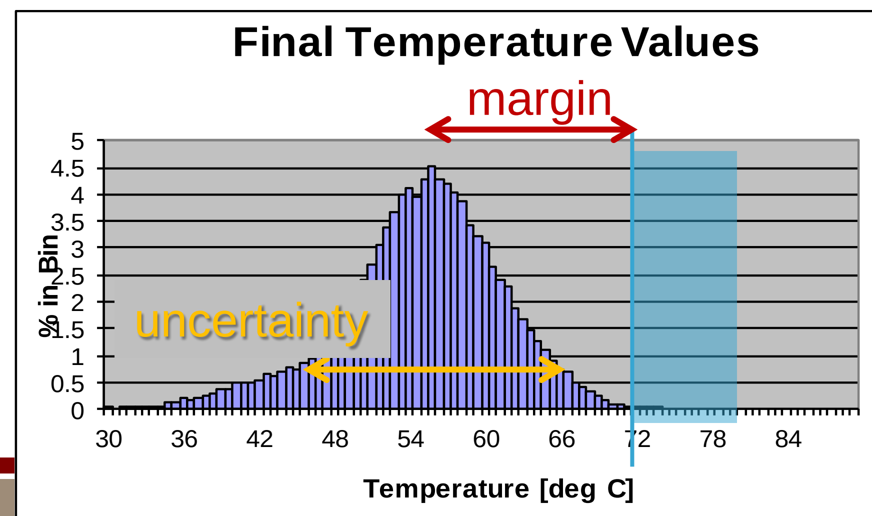


Uncertainty Quantification

- ***Given parameter uncertainty, what is the uncertainty in the model output?***
  - Mean or median performance of a system
  - Overall variability in model response
  - Probability of reaching failure/success (reliability)
  - Range/intervals of possible outcomes
- ➢ UQ also enables statistical validation metrics

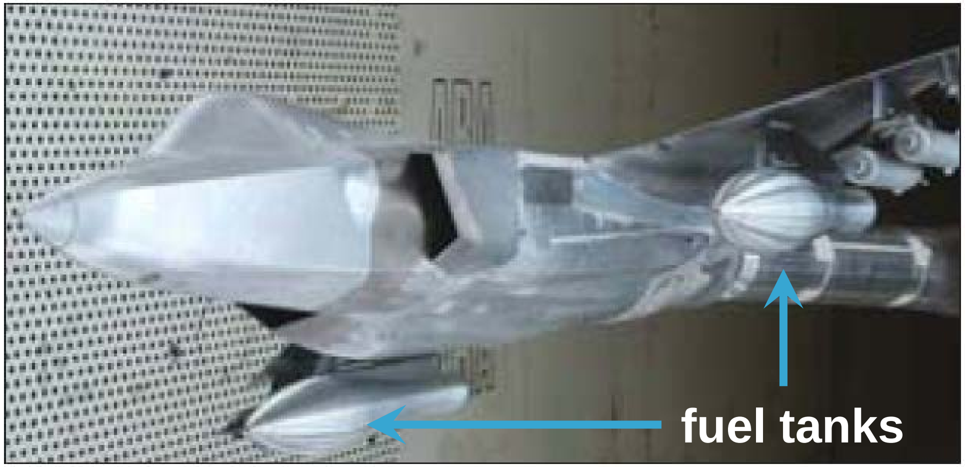


- Device subject to heating, e.g., modeled with heat transfer code
- Uncertainty in composition/ environment (thermal conductivity, density, boundary)
- Make risk-informed decisions about margin to critical temperature



Optimization

- ***Goal-oriented: find the best performing design or scenario, subject to constraints***
  - Identify system designs with maximal performance
  - Determine operational settings to achieve goals
  - Minimize cost over system designs/operational settings
  - Identify best/worst case scenarios

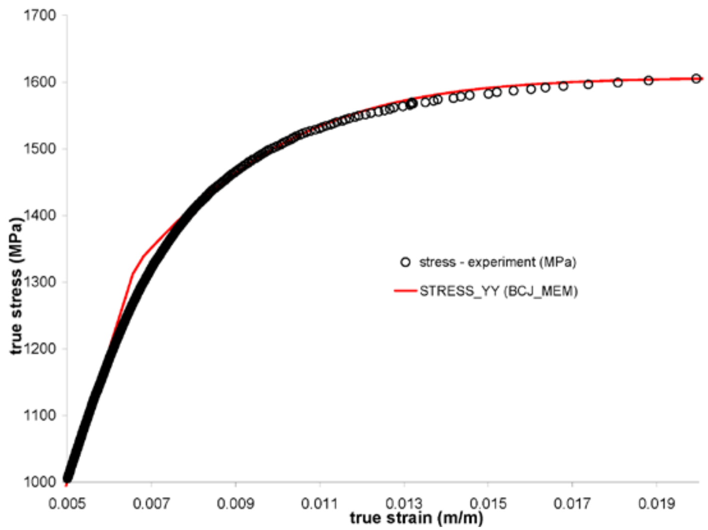


- Computational fluid dynamics code to model F-35 performance
- Find fuel tank shape with constraints to minimize drag, yaw while remaining sufficiently safe and strong

Calibration / Parameter Estimation

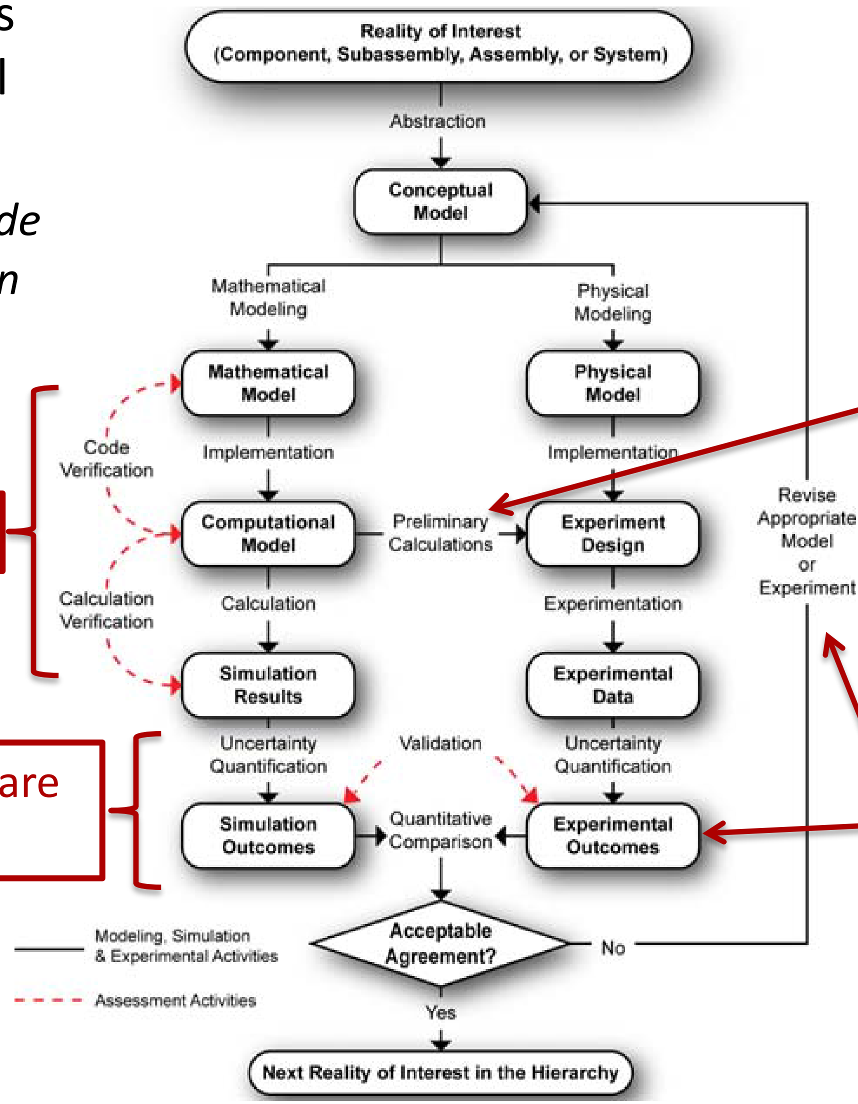
- ***Data-driven: find parameter values that maximize agreement between simulation output and experiment***
  - Seek agreement with one or more experiments,
    or high-fidelity model runs
  - Yields: single best set, range, or distribution of parameters most consistent with data

- Calibrate material model parameters to match experimental stress observations



Supports Credible Prediction

- Dakota can help with parts of a V&V workflow, crucial for credible prediction
- Example: *ASME V&V 10 Guide for Verification and Validation in Computational Solid Mechanics*



sensitivity analysis to down-select

design of computer experiments

verification

uncertainty-aware validation

calibration / comparison with data

WHY USE DAKOTA?

Dakota: Distinguishing Strengths

- Makes sensitivity analysis, optimization, and uncertainty quantification practical for costly computational models
- Flexible interface to simulation codes: one interface; many methods
- Combined deterministic/probabilistic analysis
- Continual advanced algorithm R&D to tackle computational challenges (particularly in SNL's national security mission)
  - Treats non-smooth, discontinuous, multi-modal responses
  - Surrogate-based, multi-fidelity, and hybrid methods
  - Risk-informed decision-making: epistemic and mixed UQ, rare events, Bayesian
- Scalable parallel computing from desktop to HPC

Many Methods in One Tool

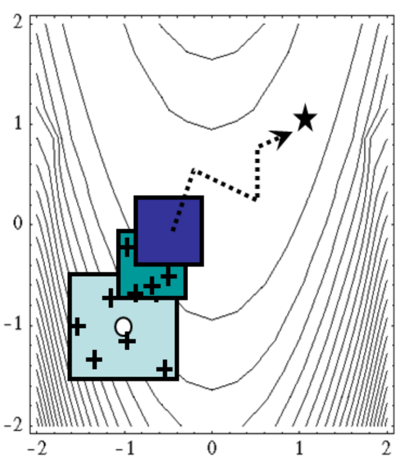
Sensitivity Analysis	Uncertainty Quantification
• Designs: MC/LHS, DACE, sparse grid, one-at-a-time • Analysis: correlations, scatter, Morris effects, Sobol indices	• MC/LHS/Adaptive Sampling • Reliability • Stochastic expansions • Epistemic methods
Optimization	**Calibration**
• Gradient-based local • Derivative-free local • Global/heuristics • Surrogate-based	• Tailored gradient-based • Use any optimizer • Bayesian inference

Interface Dakota to your simulation once, then apply various algorithms depending on your goal…

Engineering Needs Drive Dakota R&D

Advanced approaches help you solve practical problems:

- Characterize parameter uncertainty → Bayesian calibration
- Hybrid analysis → mix methods, surrogates, and models
- Mixed uncertainty characterizations → epistemic and mixed UQ approaches
- Costly simulations → surrogate-based optimization and UQ
- Build in safety or robustness → mixed deterministic/ probabilistic methods



$$
\begin{aligned}
\text{min} \quad & f(d) + W s_u(d) \\
\text{s.t.} \quad & g_l \leq g(d) \leq g_u \\
& h(d) = h_t \\
& d_l \leq d \leq d_u \\
& a_l \leq A_i\, s_u(d) \leq a_u \\
& A_e\, s_u(d) = a_t
\end{aligned}
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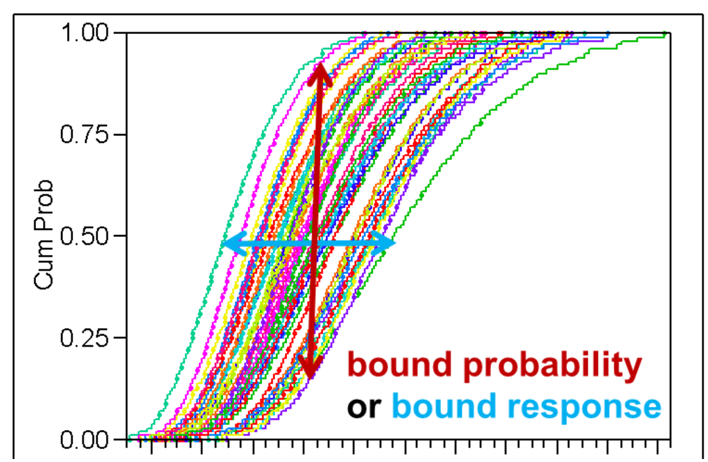
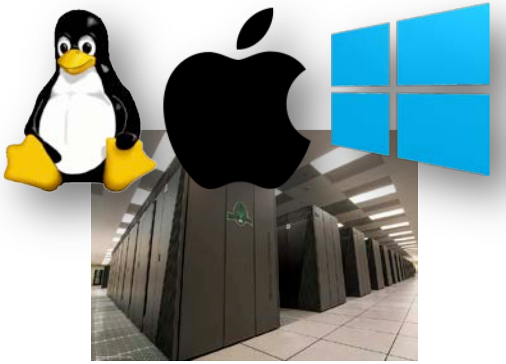
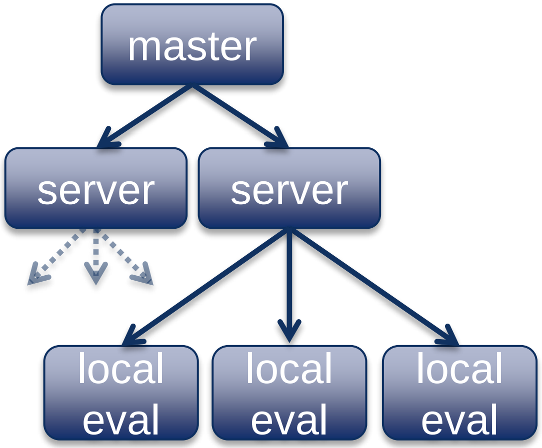


Computing and Parallelism



- Runs in various computing environments
  - Desktop: Mac, Linux, Windows
  - HPC: Linux clusters, IBM Blue Gene/P and /Q, IBM AIX, including many DOE machines
  - Distributed workstation computing
- Exploits concurrency at multiple levels
  - Multiprocessor simulations
  - Multiple simulations per response
  - Samples in a parameter study
  - Optimizations from multiple starting points
- File management features, including
  - Work directories to partition analysis files
  - Template directories share files common among analyses



Dakota History and Resources

- Genesis: 1994 optimization LDRD
- Modern software quality and development practices
- Released every May 15 and Nov 15
- Established support process for SNL, partners, and beyond

Mike Eldred, Founder

Lab mission-driven algorithm R&D deployed in production software

- Extensive website: documentation, training materials, downloads
- Open source facilitates external collaboration; widely downloaded

PREREQUISITES FOR USING DAKOTA

Intended Audience

- Primarily used by computational scientists and engineers, who work with simulations/models

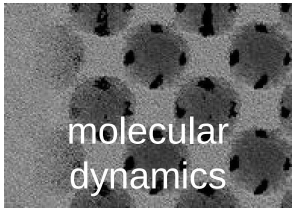
Helpful background:

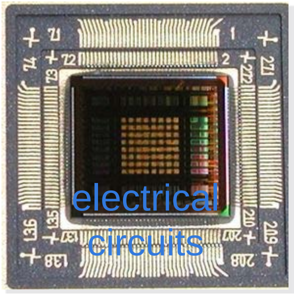
- Familiarity with mathematics, statistics, computer science
- Scripting or programming to create a Dakota-to-simulation interface
- Comfort with text-based input files and command-line interface
- Familiarity with plotting or visualization tools to post-process Dakota results

What Simulations Work with Dakota?

- Applied to many science and engineering domains:
  mechanics, structures, shock, fluids, electrical, radiation, bio, chemistry, climate, infrastructure, etc.
- Example simulation codes:
  finite element, discrete event, Matlab, Python models

- Helpful simulation characteristics:
  - Can be run in a non-interactive / batch mode
  - Parameters (inputs) not hard-wired, can be adjusted
  - Simulation responses (outputs) can be programmatically processed to extract a few key quantities of interest
  - Model is robust to parameter variations





Getting Started and Getting Help

Tour http://dakota.sandia.gov at a high level

- Getting Started
  - Download (LGPL license, freely available worldwide): http://dakota.sandia.gov/download.html
  - Getting Started: http://dakota.sandia.gov/quickstart.html
  - User's Manual, Chapter 2: Tutorial with example input files http://dakota.sandia.gov/sites/default/files/docs/6.2/Users-6.2.0.pdf

- Getting Help
  - Extensive documentation (user, reference, developer): http://dakota.sandia.gov/content/manuals
  - Support mailing list (reaches Dakota team and user community): dakota-users@software.sandia.gov

SUPPLEMENTAL SLIDES

Related Tools

Similar/Related Capabilities

- NASA UQTools
- OpenTURNS
- LLNL PSUADE
- MIT MUQ
- SNL UQTk
- OpenMDAO
- COIN-OR
- NLOpt
- Nessus, GoldSim

Often Used with Dakota

- Matlab, Python, Perl, Shell, C, C++ for interfacing
- Matlab, Excel, JMP, Minitab for post-processing and analysis

How related tools compare to Dakota

Software	Methods	Simulation Interface	Hybrid Analyses	R&D	Parallel Computing
NASA UQTools	UQ	???	no	no	???
OpenTURNS	UQ	???	no	no	no
LLNL PSUADE	SA	yes	no	no	???
MIT MUQ	UQ, Opt	custom	no	yes	no
SNL UQTk	UQ, Cal	yes	no	yes	no
OpenMDAO	Opt	yes	no	yes	yes
COIN-OR	Opt	no	no	yes	some
NLOpt	Opt	yes	no	no	no
Nessus	UQ	yes	no	???	no
GoldSim	UQ	???	no	???	no
PEST	Cal	yes	no	???	yes