Dakota Software Training

Dakota Overview

http://dakota.sandia.gov
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

<table>
<thead>
<tr>
<th>Run</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.814</td>
<td>91.3</td>
</tr>
<tr>
<td>2</td>
<td>0.906</td>
<td>63.24</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>1.270</td>
<td>9.75</td>
</tr>
</tbody>
</table>

resistances, via diameters

voltage drop, peak current

material props, boundary, initial conditions

temperature, stress, flow rate

Xyce, Spice Circuit Model

Abaqus, Sierra, CM/CFD Model
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 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*

![Diagram](image-url)
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

<table>
<thead>
<tr>
<th>Sensitivity Analysis</th>
<th>Uncertainty Quantification</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Designs: MC/LHS, DACE, sparse grid, one-at-a-time</td>
<td>• MC/LHS/Adaptive Sampling</td>
</tr>
<tr>
<td>• Analysis: correlations, scatter, Morris effects, Sobol indices</td>
<td>• Reliability</td>
</tr>
<tr>
<td></td>
<td>• Stochastic expansions</td>
</tr>
<tr>
<td></td>
<td>• Epistemic methods</td>
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</table>

<table>
<thead>
<tr>
<th>Optimization</th>
<th>Calibration</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Gradient-based local</td>
<td>• Tailored gradient-based</td>
</tr>
<tr>
<td>• Derivative-free local</td>
<td>• Use any optimizer</td>
</tr>
<tr>
<td>• Global/heuristics</td>
<td>• Bayesian inference</td>
</tr>
<tr>
<td>• Surrogate-based</td>
<td></td>
</tr>
</tbody>
</table>
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

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

http://dakota.sandia.gov
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 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

<table>
<thead>
<tr>
<th>Software</th>
<th>Methods</th>
<th>Simulation Interface</th>
<th>Hybrid Analyses</th>
<th>R&amp;D</th>
<th>Parallel Computing</th>
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