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Dakota: Advanced Exploration of Simulations

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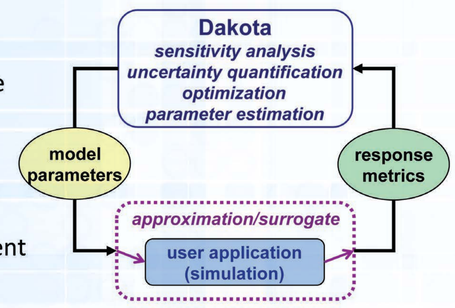
Objective: Enable advanced exploration of science and engineering simulations

- Apply sensitivity analysis, UQ, optimization, and calibration to computational models
- Facilitate design trade-offs, V&V, QMU, risk-based decision making

- Non-intrusive iterative systems analysis
- Parallel computing: desktop to HPC
- Simulation management



Open source to facilitate research collaboration

- Genesis in 1994 optimization LDRD
- Extensive website, documentation, and training materials
- LGPL; 11,000+ downloads registered
- Currently 12 core SNL contributors
- Key external collaborators:

Vanderbilt University · Los Alamos National Laboratory · USC University of Southern California · CASL · Stanford · The University of Texas at Austin

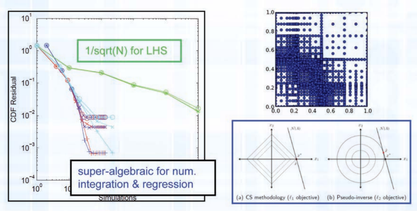
UQ research targets engineering challenges

Challenges

- Limited simulation budgets
- Many random variables
- Mixed epistemic/aleatory
- Low probability events
- Non-smooth responses

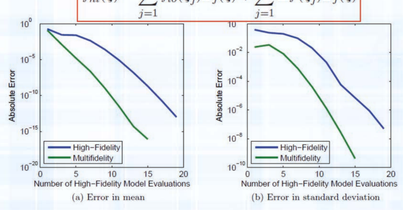
Capability Highlights

- Goal-oriented adaptive refinement
- Sparsity detection
- Multi-fidelity; leverage lo-fi
- Interval-based epistemic/aleatory
- Efficient Bayesian calibration, optimization under uncertainty

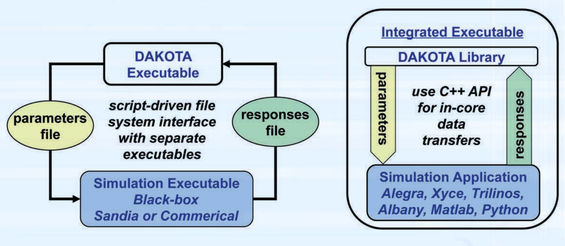


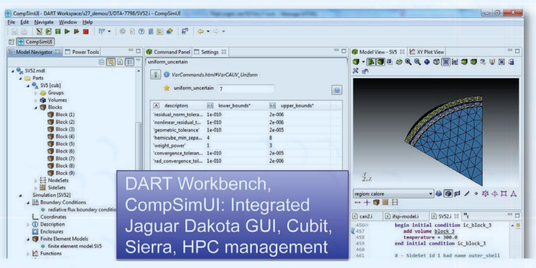
Target discrepancy between hi-fi and lo-fi

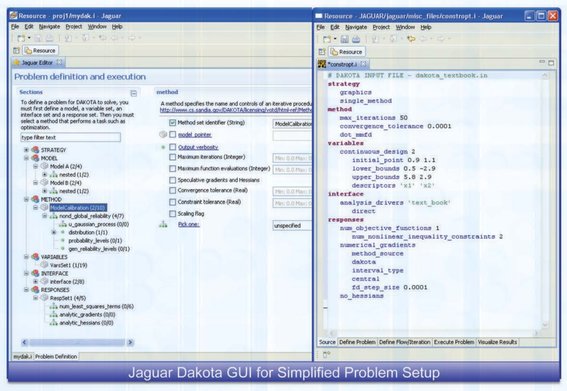
$$\hat{f}_{hi}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$



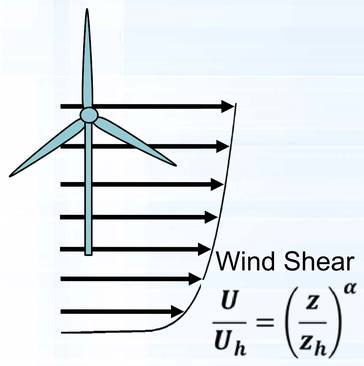
Deliver in engineer's environment to gain efficiency and usability

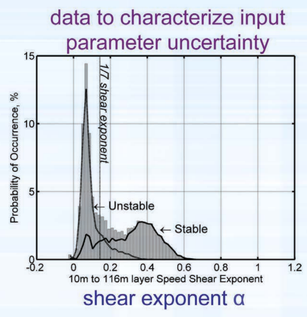


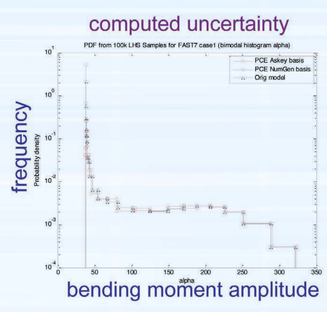




Effect of uncertain shear on wind turbines

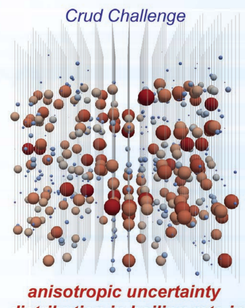






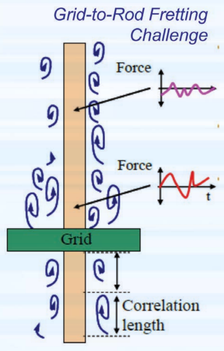
- Propagate histogram uncertainty with Dakota and NREL's FAST aero-elastic code

CASL: V&V/UQ for nuclear engineering



anisotropic uncertainty distribution in boiling rate in quarter core model

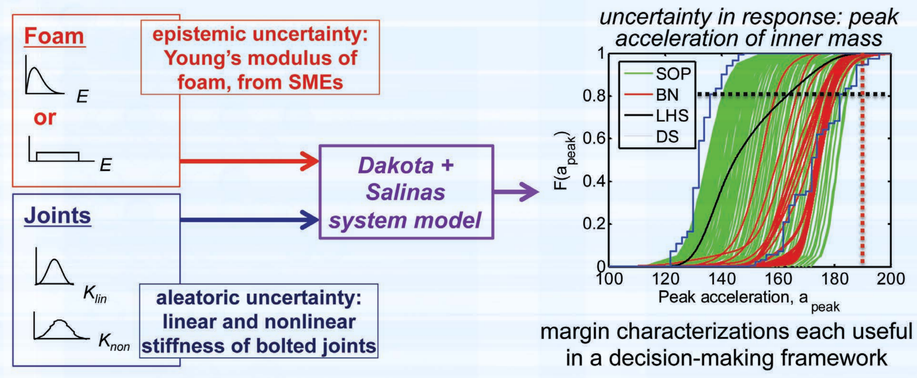
- Dakota central to CASL's Virtual Reactor
- Verification, validation, calibration, sensitivity, uncertainty analyses for reactor core
- Multi-physics motivates algorithm development



Broad use for NW applications

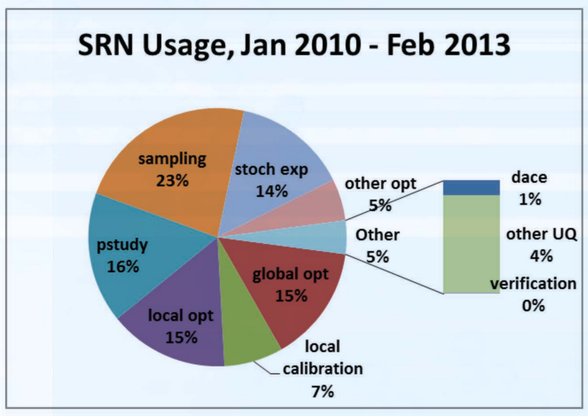
- Supports ALTs and LEPs, as well as AAR
- Calibration, V&V, UQ across components and systems
- Structural, mechanical, thermal, radiation, electrical models

System-level aerospace structural dynamics QMU:



margin characterizations each useful in a decision-making framework

Summary: Dakota broadly impacts Sandia's engineering mission



49543 *tracked* invocations by 146 unique users; high HPC demand

- Engineering challenges guide investments
- Research collaborations ensure competitiveness
- Proactive deployment and partnering: adoption and impact of advanced algorithms

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