SAND2017-2170C

DAKOTA

Explore and predict with confidence

CCR

Center for Computing Research

Algorithms for Design Exploration and Simulation Credibility

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Optimization and Uncertainty Quantification

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Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

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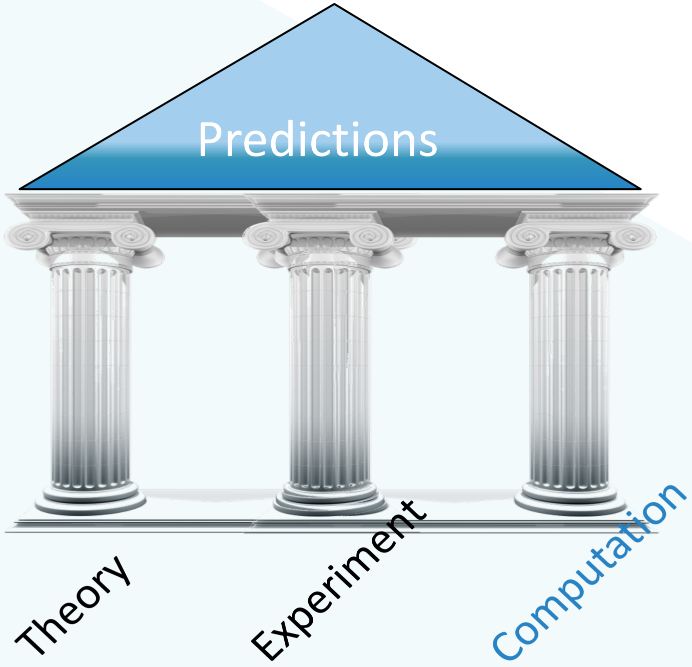
Credible Prediction in Scientific Discovery and Engineering Design



- Computational models, enabled by theory and experiment, can help:
  - Predict and analyze scenarios, including in untestable regimes
  - Assess risk and robustness
  - Design through virtual prototyping
  - Generate or test theories
  - Guide physical experiments
- *Answer what-if? when experiments infeasible…*

For simulation to credibly inform scientific, engineering, and policy decisions we must:

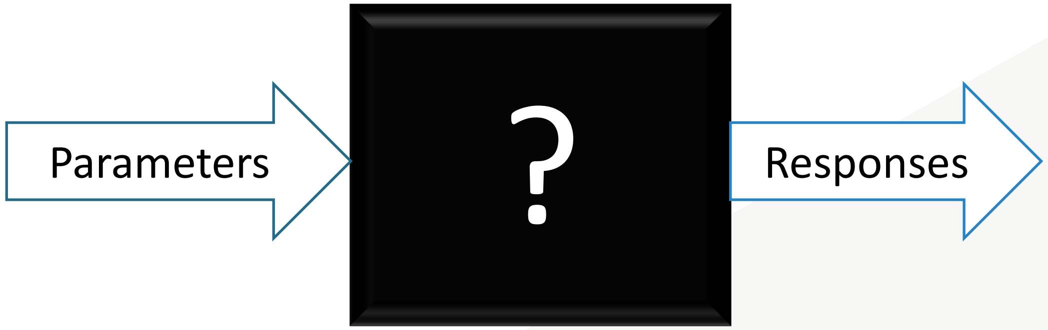
- Ask critical questions of theory, experiments, simulation
- Identify and characterize sources of uncertainty and their consequences
- *Create reliable tools for design and exploration, and facilitate adoption of those tools by science and engineering practitioners*

Black-Box Design Exploration using Dakota

The Dakota toolkit is one such tool.

- Dakota employs a **black-box approach** to make sophisticated parametric exploration of simulations **practical** and **accessible** for a computational design-analyze-test cycle.
- Dakota is:
  - A suite of iterative mathematical and statistical methods for sensitivity analysis, uncertainty quantification, model calibration, and optimization.
  - Facilities for interfacing these algorithms with arbitrary computational models/simulations.
- Dakota orchestrates and analyzes ensembles of simulations to aid discovery of the best designs, the most important variables, and the consequences of uncertainty.

Black-box approach: What is it?



Simulation

- Parameters are mapped through a simulation to responses without regard for simulation internals.
- In particular, no *access to* or *knowledge of* the simulation's source code or underlying data structures is needed: Algorithms are coupled to inputs and output via the ordinary user interface
- Algorithms are not specialized to physics or simulation technique

Advantages of a Black-Box approach

Compared to more tightly-coupled or intrusive techniques, a black-box approach can offer time and resource advantages when:

- User has no access to the simulation source code: simulation is closed-source, or modification is disallowed by licensing or policy, etc.
- User lacks expertise to modify the source.
- The costs associated with modifying the simulation are prohibitive.

… Situations that frequently arise for science and engineering practitioners.

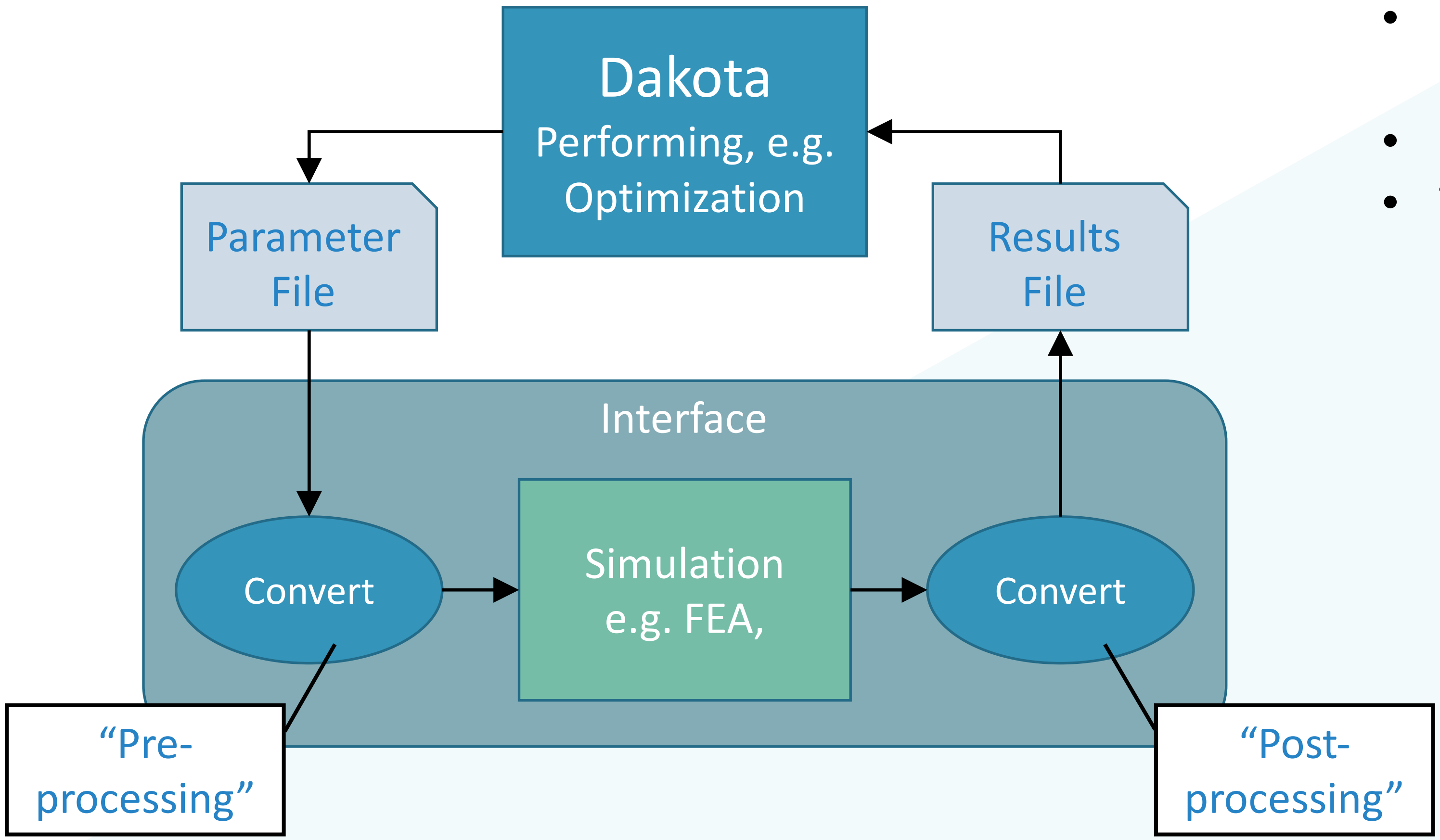
Dakota

- Developed continuously since 1994, primarily at Sandia National Laboratories
  - Significant ongoing support from DOE and other sources
- Open Source
  - LGPL license
- Modern software development practices
  - Agile planning, continuous integration
- Incorporates many third-party libraries
- Deployment vehicle for algorithms research, which is strongly informed by needs at the Labs and elsewhere

Mike Eldred, Founder

Dakota-Simulation Interfacing

Interfacing between Dakota and computational models is file-based



- User develops the interface between Dakota and the simulation
- Can be in any language
- Typically quite simple and flexible!

For each evaluation of the sim, Dakota

1. Writes a parameters file
2. Invokes the user's interface
3. Reads the results file

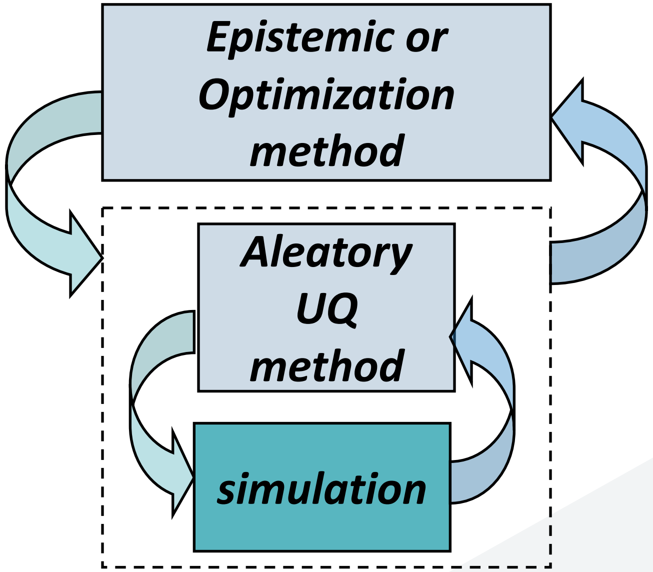
Diversity of Algorithms

Sensitivity Analysis	Uncertainty Quantification
• Sampling, classical designs, parameter studies • Results: Correlations, Morris effects, Sobol' indices	• MC/LHS/Adaptive Sampling • Reliability • Stochastic expansions • Epistemic methods
Optimization • Gradient and non-gradient local • Global/heuristics and multiobjective • Surrogate-based	**Calibration** • Tailored gradient-based • Use any optimizer • Bayesian inference

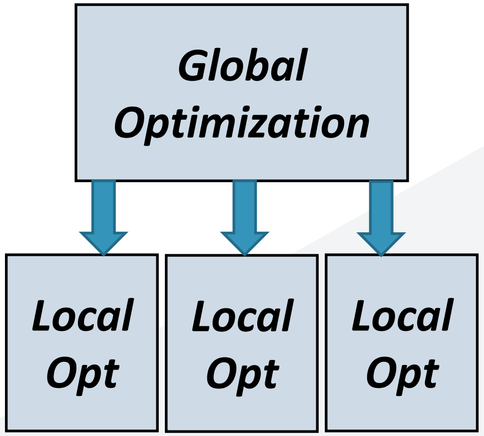
- Once a Dakota-Simulation interface is created, any algorithm can be applied with minimal or no changes.
- Ease of switching algorithms facilitates experimentation and multistage workflows.

Other Capabilities

Mixed UQ or Optimization under Uncertainty



Sequential Optimization



- Advanced strategies support nesting and combining methods
- Dakota itself is MPI parallelized to take advantage of available concurrency

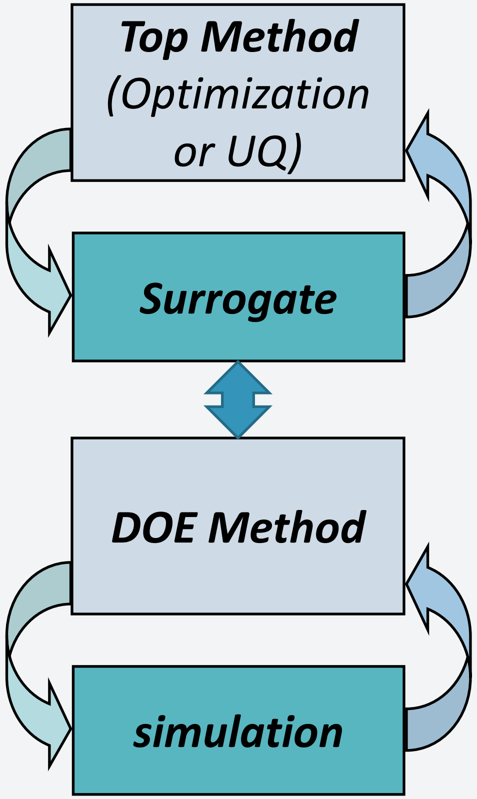
Surrogate Models

Surrogate models can be constructed, used, and exported for later evaluation

- Polynomial
- Gaussian Process
- Many others
- Piecewise Surrogates

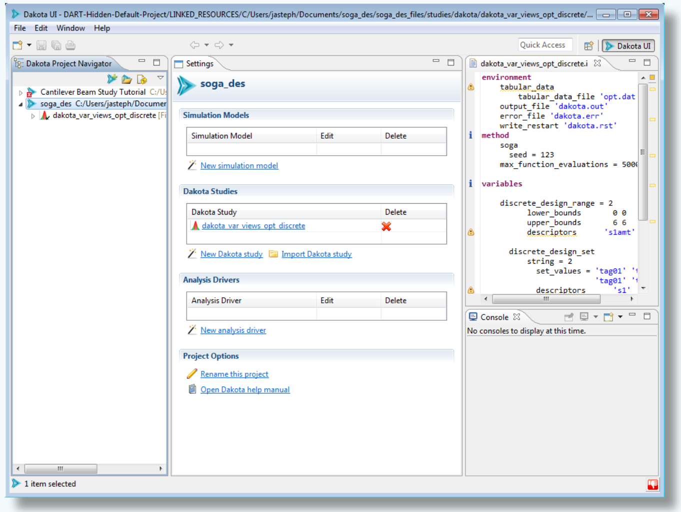
New to Dakota:

- Active subspace
- Random fields



Where Dakota is Going

New User Interface



Current & Anticipated Features

- Goal-oriented study wizards
- Automated interfacing
- Plotting
- Run management
- Context-sensitive help

Algorithms Research

- Multilevel-Multifidelity UQ *(MS70: Eldred, Monschke, Jakeman, Geraci)*
- Model-form error in Bayesian Calibration *(MS51: Farrell-Maupin, Swiler)*

Five-Year Strategic Plan

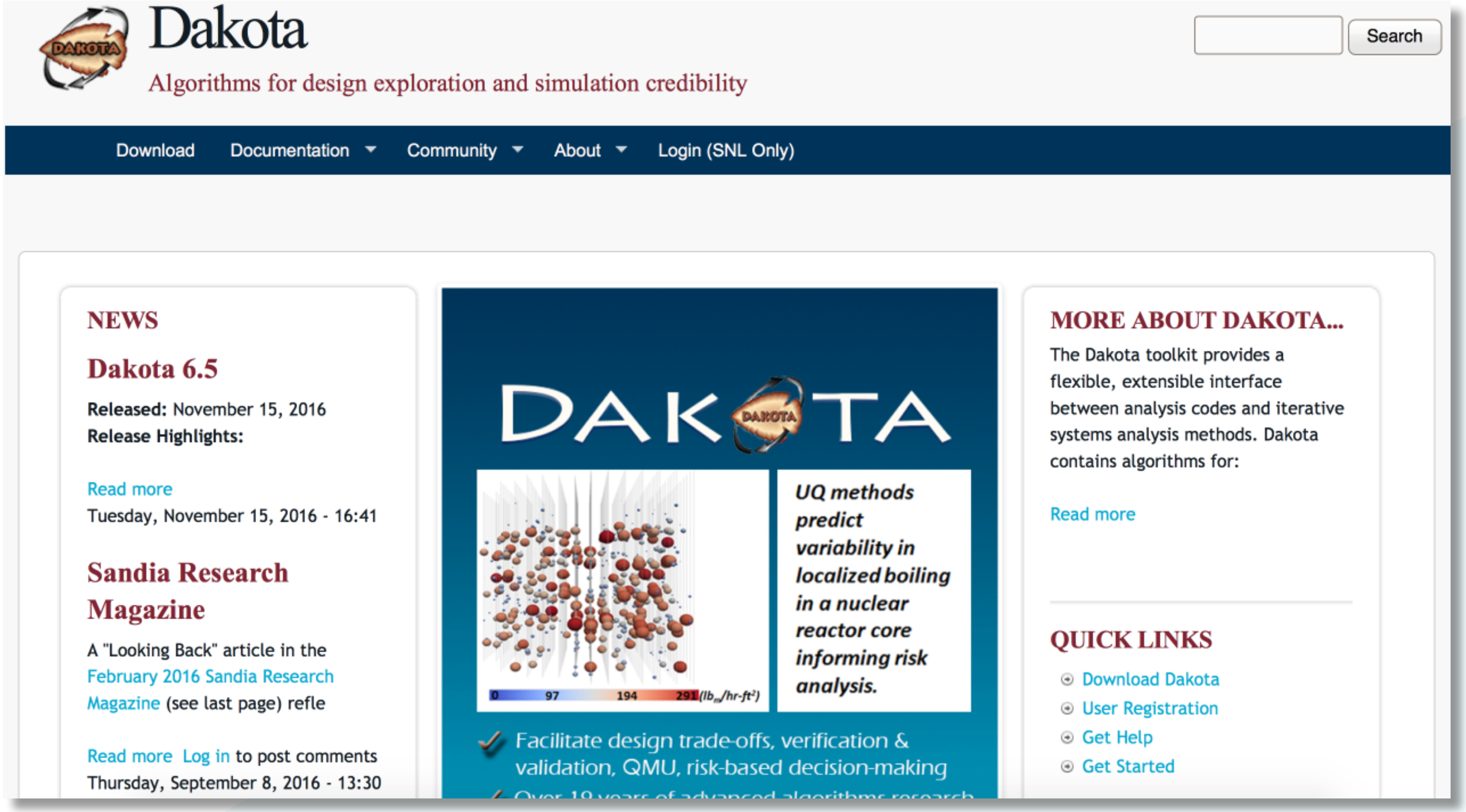
Select Outcomes

- Transformation into a modular, extensible system of components
- Active and educated user community

Other Tools

Name	Developer/Sponsor	Open Source?	Type	Capabilities
UQTools	NASA	N	Matlab Toolbox	UQ
OpenTURNS	Industry Partners	Y	Python Library	UQ, SA, Surrogates
PSUADE	LLNL	Y	C++ Library and Executable	UQ, SA, Surrogates
MUQ	MIT	Y	C++ Library	Optimization, UQ, Surrogates
UQTk	SNL	Y	C++ Library	UQ, SA
OpenMDAO	NASA	Y	Python Library	Optimization
NLOpt	Community	Y	C Library (many wrappers)	Optimization
Nessus	SwRI	N	GUI-Based	Reliability and UQ
SMARTUQ	SMARTUQ	N	GUI-Based	UQ, SA

Resources



https://dakota.sandia.gov

On the Portal

- Source and downloads
- Examples
- dakota-users mailing list
- Extensive documentation
- Training videos with exercises

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