SAND2018-5144 C

Exceptional service in the national interest

Dakota Optimization and UQ

Explore and Predict with Confidence

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Optimization and Uncertainty Quantification

Patricia D. Hough

Quantitative Modeling and Analysis

http://dakota.sandia.gov

2018 SIAM Conference on Uncertainty Quantification
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Garden Grove, CA

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SNL Mission: Advanced Science and Engineering for National Security

- Nuclear Weapons
- Defense Systems and Assessments
- Energy and Climate
- Global Security

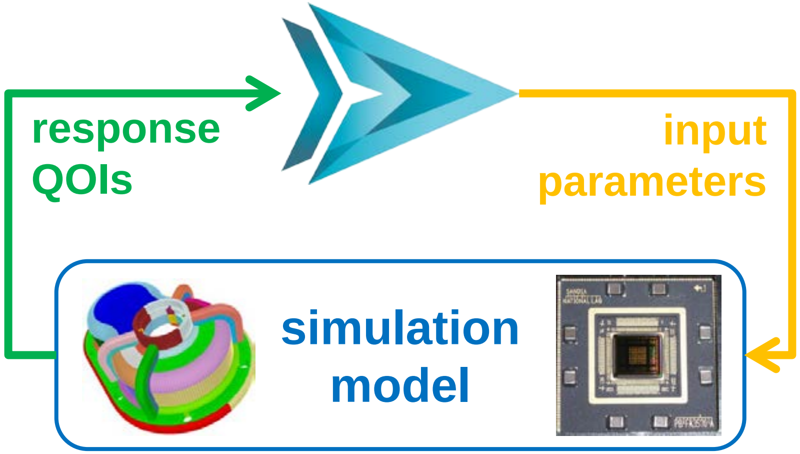
Strong research foundations span many disciplines

Dakota Mission:
To serve Sandia's mission through state-of-the-art research and robust, usable software for optimization and uncertainty quantification.

Dakota Team: has balanced strengths in algorithm research, software design and development, and application deployment and support

Dakota: Algorithms for Design Exploration and Uncertainty Quantification

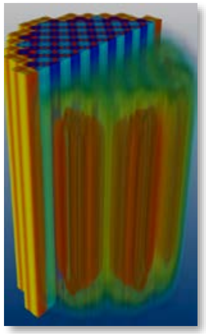
- Suite of iterative mathematical and statistical methods that interface to computational models
- Makes sophisticated parametric exploration of black-box simulations practical for a computational design-analyze-test cycle:
  - Sensitivity Analysis
  - Uncertainty Quantification
  - Design Optimization
  - Model Calibration



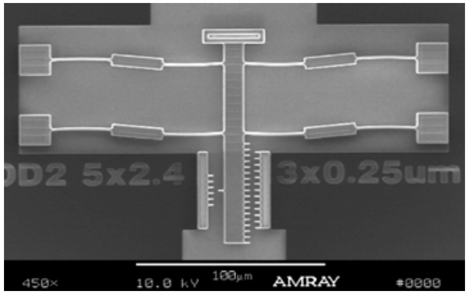
- *Goal: provide scientists and engineers (analysts, designers, decision makers) richer perspective on model predictions*

Practical Design Exploration and UQ for Diverse Simulations

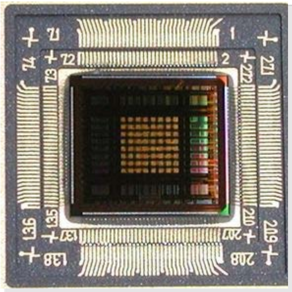
- **Applied to many science and engineering domains**
  mechanics, structures, shock, fluids, electrical, radiation, bio, chemistry, climate, infrastructure, etc.
- **Diverse, often costly, simulation codes:**
  finite element, coupled multi-physics, discrete event, Matlab, Python models



UQ and Bayesian inference for nuclear reactor core analysis



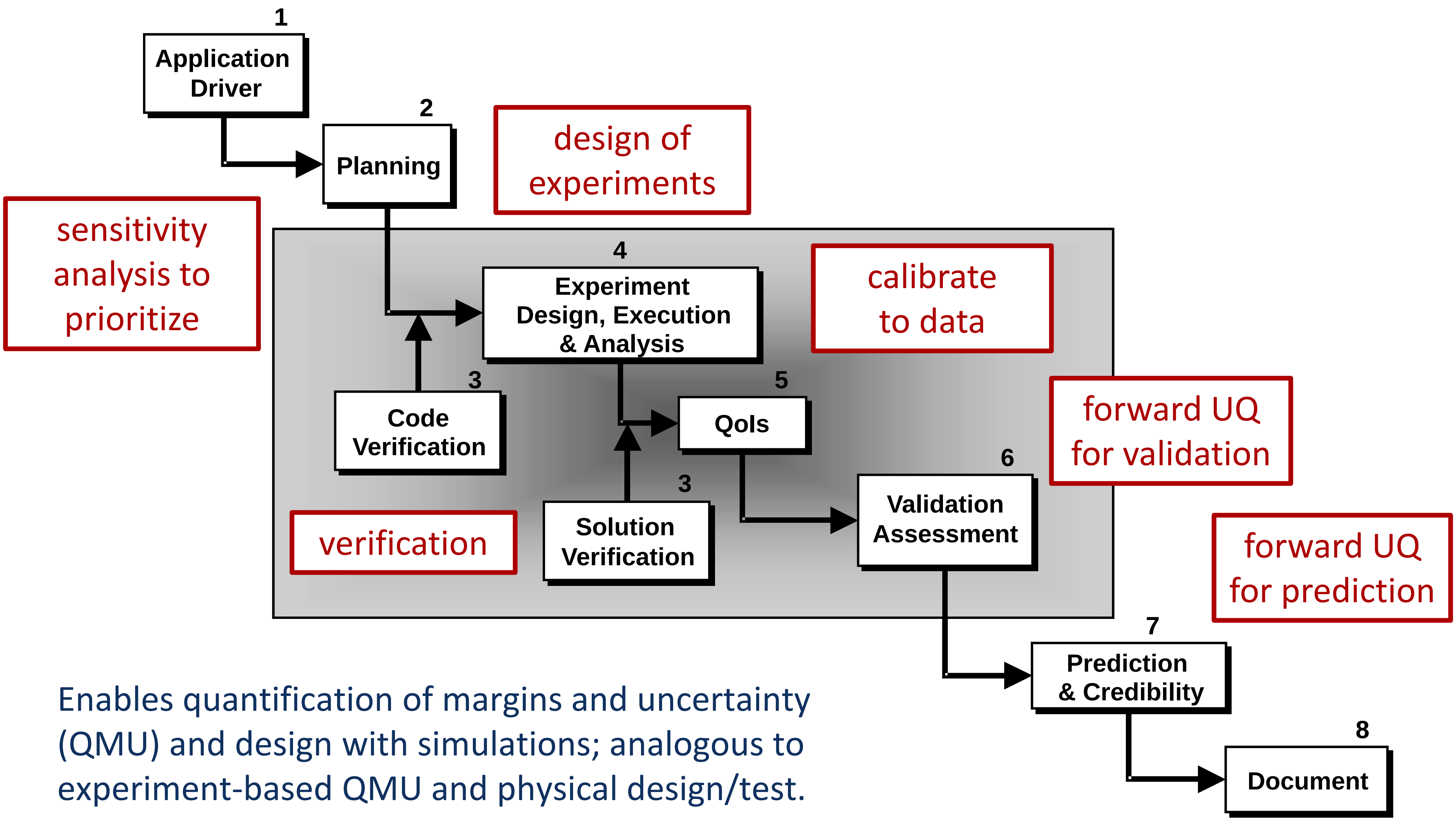
Reliability-based design optimization of micro-electro-mechanical systems (MEMS)



UQ for qualification of electrical circuits in harsh environments

Adjoint-based UQ for robust design of satellite radiation shields

Supports Credible Prediction



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

Many Methods in One Tool

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Sensitivity Analysis • Designs: param. sweeps, MC/LHS, DACE, sparse grid, one-at-a-time • Analysis: correlations, scatter, Morris effects, Sobol indices	**Uncertainty Quantification** • MC/LHS/Adaptive sampling • Local/global reliability • Stochastic expansions • Epistemic and interval methods • Multi-fidelity/multi-level
Optimization • Gradient-based local • Derivative-free local • Global/heuristics • Surrogate-based, multi-fidelity	**Calibration** • Tailored gradient-based • Use any optimizer • Bayesian inference

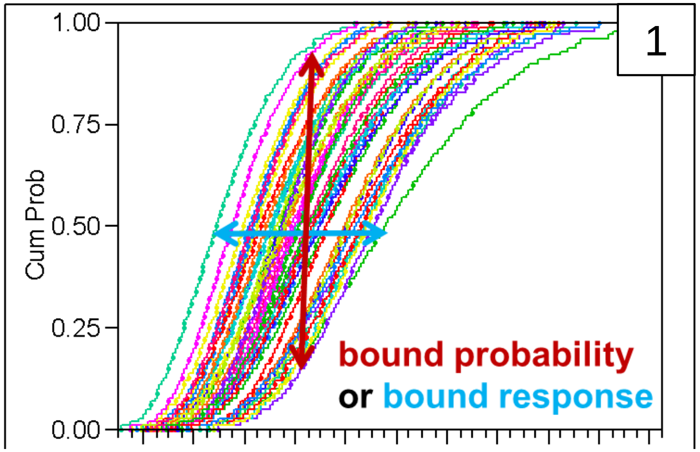
✓ One flexible simulation interface, many methods: once interface created, apply appropriate algorithm depending on question at hand

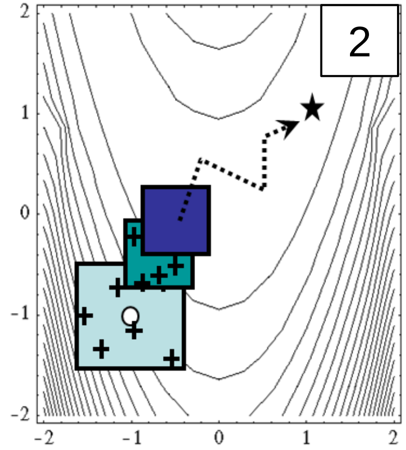
✓ Scalable parallel computing from desktop to HPC

Engineering Needs Drive Dakota R&D

Advanced approaches help you solve practical problems:

- Characterize parameter uncertainty → Bayesian calibration
- Hybrid analysis goals → mix methods, surrogates, and models
- Mixed uncertainty characterizations → epistemic and mixed UQ approaches [1]
- Costly or noisy simulations → surrogate-based optimization [2] and UQ
- Build in safety or robustness → mixed deterministic/probabilistic methods [3]





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

Dakota History and Resources

- Genesis: 1994 optimization LDRD
- Modern software quality and development practices
- Released every May 15 and Nov 15
- Established user support process and mailing list

Mike Eldred, Founder

http://dakota.sandia.gov

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

- Extensive website: documentation, training slides/videos, downloads
- Open source to facilitate collaboration; widely downloaded

Dakota Capability Directions

2016—2020 Strategic Plan stewards Dakota's research program while improving production deployment and impact

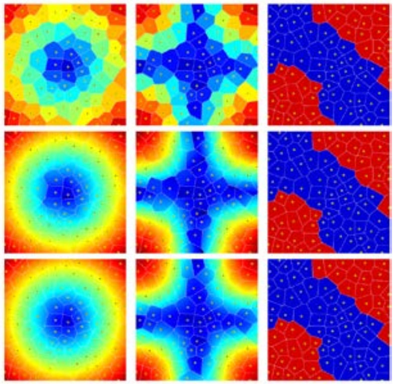
R&D Challenges

Tackle design exploration and UQ computational challenges
(focusing on DOE national security mission):

- Severely constrained simulation budgets
- High-dimensional parameter spaces
- Non-smooth, multi-modal, or unreliable quantities of interest
- Quantifying small probabilities

Active Algorithm R&D

- Core UQ: robust, scalable, adaptive sampling and stochastic expansions
- Multi-fidelity, multi-level optimization, inference, UQ methods
- Calibration: usable, robust deterministic and Bayesian methods
- Optimization: new gradient-based and discrete optimization methods
- Algorithms and interfaces that directly treat functional (time/space) data
- Scalability in number of parameters / responses and to next-generation architectures and parallelism models
- Reduced-order models: surrogates, active subspace, random field models



Discontinuity-detecting piecewise local surrogate models (Ebeida)

Multi-level/Multi-fidelity Methods

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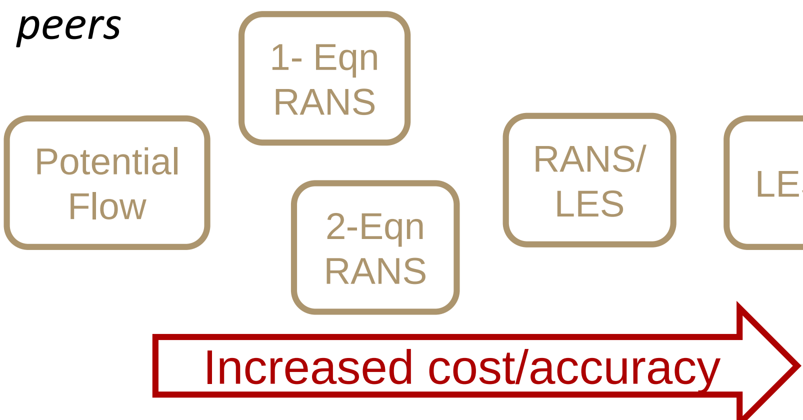
Goal: Use models of varying fidelities and/or levels to converge more quickly

- ML/MF sampling, stochastic expansions, optimization, calibration
- Automatically balance evaluations of each model

Multi-level: hierarchy of numerical approximation accuracies, *e.g., mesh resolution, solver tolerance*

Multi-fidelity: physics model detail; *hierarchy or peers*



fidelity ↓ / level →			
	$ 1000's	$$ 100's	$$$ 10's
	$$ 100's	$$$ 10's	$$$$ 1

See talks by Eldred, Geraci

Inference: Bayesian Calibration

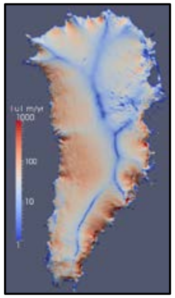
Goal: Obtain statistical characterization of parameters consistent with data

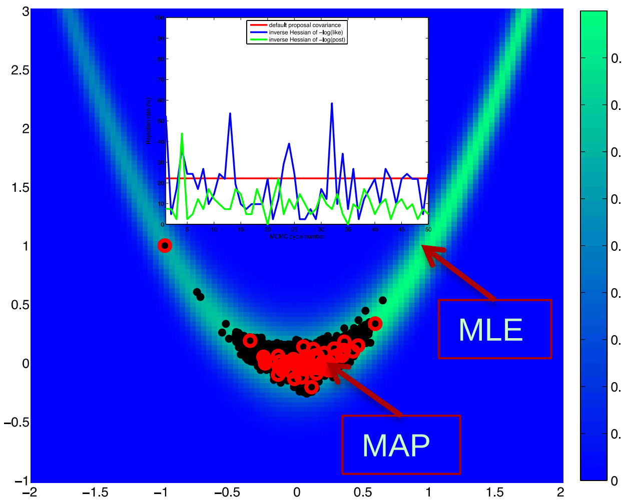
- MCMC with QUESO/DRAM and DREAM
- Adaptive, surrogate-based inference, including with ML/MF PCE
- Mutual information guided calibration of low-fi to high-fi model
- Usability: chain post-processing, statistics, credible/prediction intervals, KDE-smoothed posteriors, mutual information

Emerging capabilities

- Discrepancy models
- Metropolis-adjusted Langevin Algorithm
- Non-MCMC-based approaches
- Automated diagnostics and filtering
- Coupling with forward UQ methods

See talks by Jakeman, Maupin, Perego, Wildey





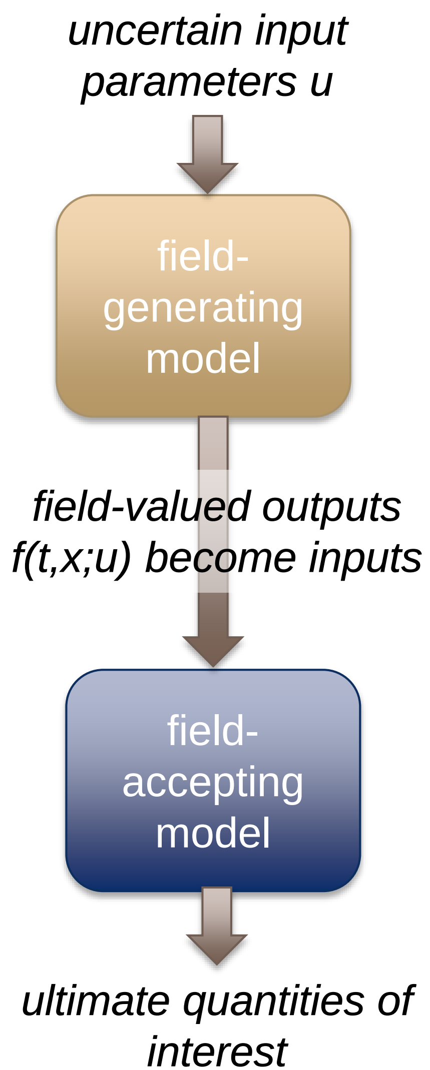
Random Field Modeling

Goal: perform UQ with field-valued (time- or space-varying) input uncertainties *f(t, x)*, e.g., boundary conditions

- Generate realizations of *f(t; u)*: either sample the field-generating model or use offline data
- Approximate uncertainty in *f(t; u)*, e.g., by PCA + GP, or a Karhunen–Loève expansion with normal coefficients ω

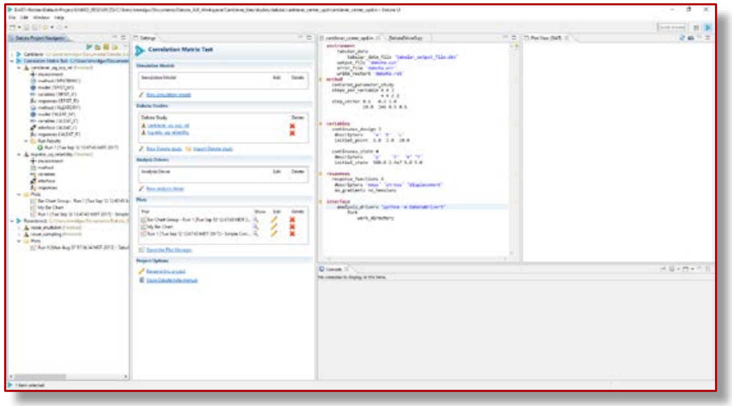
$$\hat{\boldsymbol{f}}(t,\omega) = \boldsymbol{\mu_f}(\boldsymbol{t}) + \sum_{i=1}^{P} c_i(\omega)\,\varphi_i\ (t)$$

- Propagate: perform UQ over ω, generating realizations of the approximate field $\hat{\boldsymbol{f}}(t,\omega)$ and propagate through the field-accepting model



Other Development Areas

- Modular architecture
  - Ease Dakota development and give greater control to advanced users
  - Example 1: Surrogate model
  - Example 2: Optimizer traits and APIs



- Usability and user resources
  - Example 1: GUI
  - Example 2: Output database
  - Example 3: `dakota.interfacing` Python module
  - Example 4: Examples repo

- Improved user community engagement
  - Example 1: Dakota user-stakeholder meetings
  - Example 2: Surveys and interviews

DAKOTA

Explore and predict with confidence

http://dakota.sandia.gov

Thanks for your attention!

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Other team members presenting at SIAM UQ:
Eldred, Geraci, Jakeman, Khalil, Maupin, Swiler

BACKUP (ADDITIONAL DETAILS)

HPC Integration

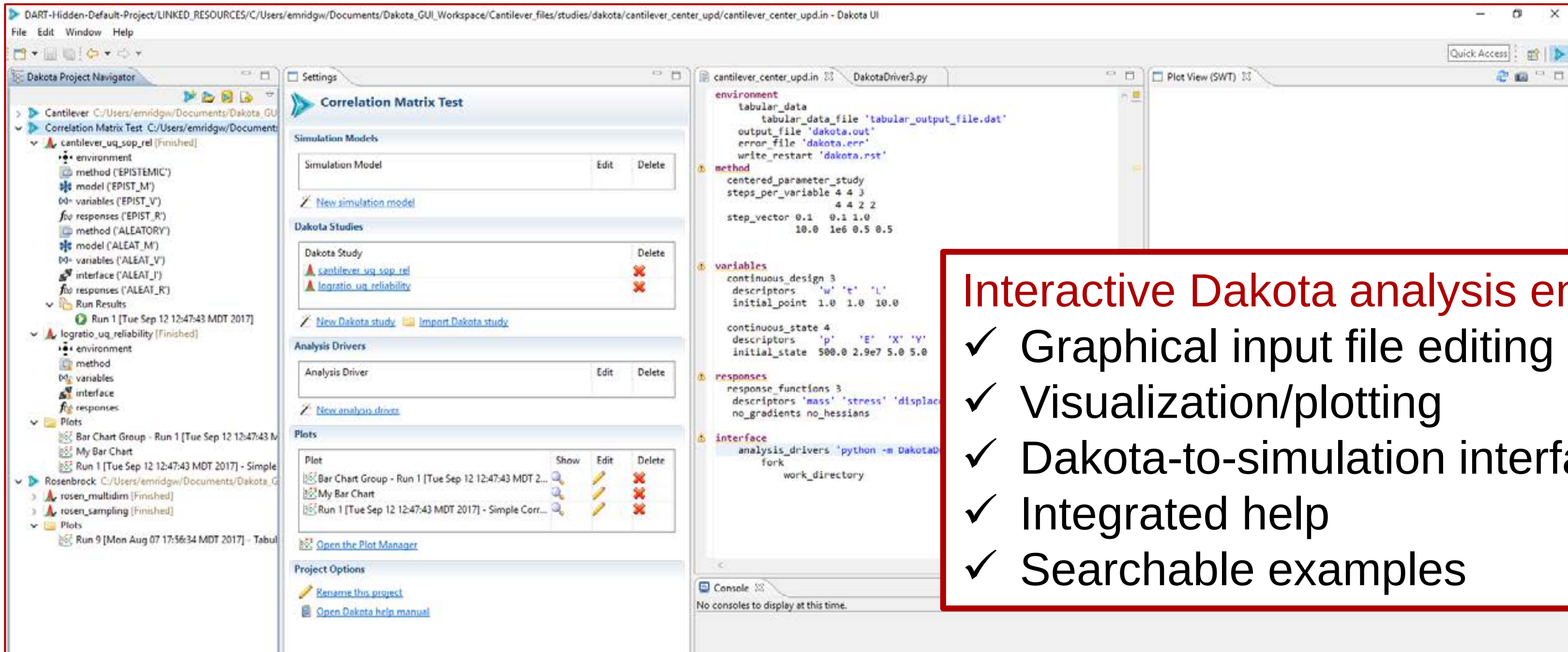
Dakota readily integrates into HPC environments

Massively Serial	Evaluation Tiling	Evaluation Submission
Dakota runs in parallel and drives a large number of serial simulations	Dakota runs serially as part of a submitted job and "tiles" intermediate-sized parallel simulations across the job	Dakota runs serially on the login node and submits large parallel simulations as separate jobs.

Three common use cases

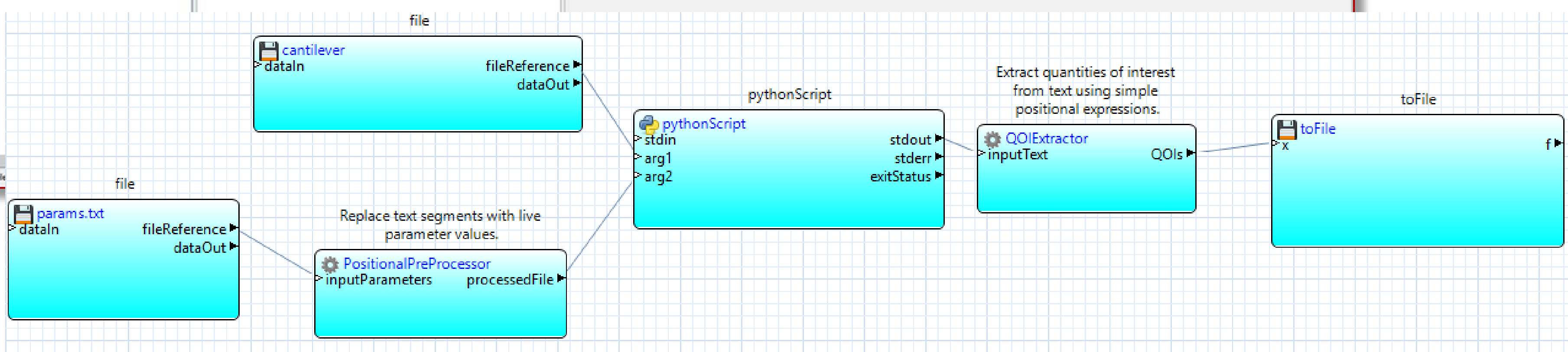
- ➢ Example interface scripts provided
- ➢ Python modules in development

Graphical User Interface



Interactive Dakota analysis environment

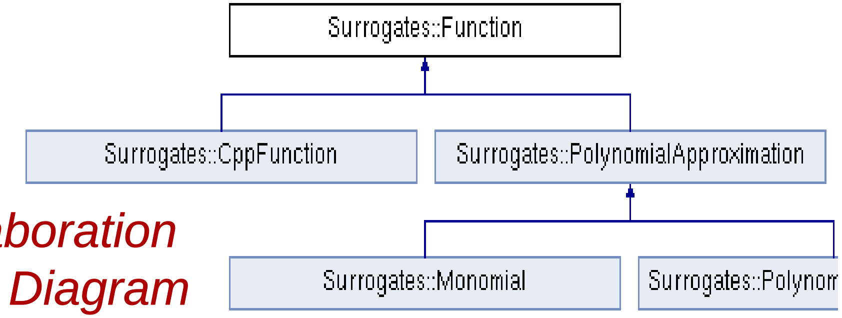
- ✓ Graphical input file editing
- ✓ Visualization/plotting
- ✓ Dakota-to-simulation interface wizard
- ✓ Integrated help
- ✓ Searchable examples



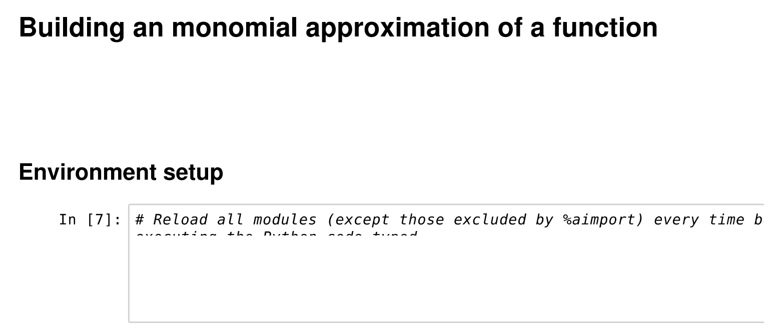
Dakota Modularization: Surrogate Model Library

Initial prototype demonstrated

- Modularize foundational utilities and surrogate models
- Progress on unifying Dakota, Surfpack, Pecos
- Increasing unit testing, coverage, and software quality
- Python interfaces to C++ components for ease of use by advanced users
- Jupyter-based interactive Python tutorial demonstrates more usable coordination of model components with Python



Collaboration Diagram



iPython Notebook

dakota.interfacing

Tools for Python-based black-box simulation interfacing

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- Read params files/write results files

```python
#!/usr/bin/env python

import dakota.interfacing as di
from rosenbrock import rosenbrock_function

params, results = di.read_parameters_file()

x1 = params['x1']
x2 = params['x2']

results['f'].function = rosenbrock_function(x1, x2)

results.write()

```

- Evaluation tiling helper

```bash
#!/bin/bash

params=$1
results=$2

# For dynamic scheduling:
mpitile -np 2 text_book_simple_par $params $results

```

TODO

- ❑ Evaluation Submission helpers
- ❑ Template substitution
- ❑ Integration into GUI

Promote User and Development Community Engagement

- Web resources:
  - Interactive user forums
  - Capability maturity ratings and test linkage
  - Community repository of code, examples, scripts
- Training materials: presentations, videos, exercises
- New graphical user interface for Dakota analysis

- Improved modularity so users can extend, contribute components, e.g.,
  - Surrogate model module with Python bindings
  - More usable simulation interfacing that encourages best practices
- Communicate development practices to encourage contribution, e.g., principles, code standards, easier build/test on new platforms

- Portability to and scalability on new high-performance computers

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