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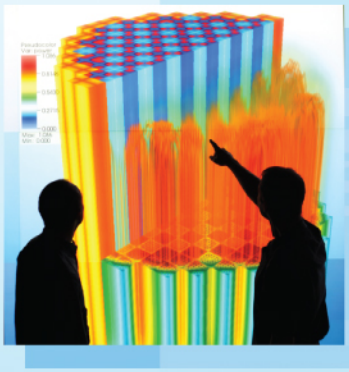
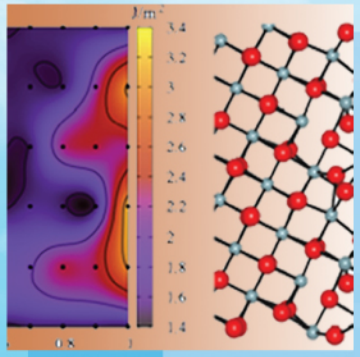
Power uprates
and plant life extension



Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

# Level 3 Milestone Deliverable – L3.VUQ.V&V.P8.01

# VUQ Milestone Review

Brian Adams and Russell Hooper
Sandia National Laboratory

Ralph Smith
North Carolina State University

Brian Williams
Los Alamos National Laboratory

March 31, 2014

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

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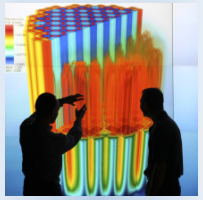
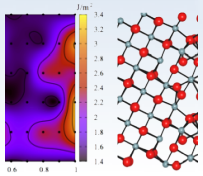




# User Guidelines and Best Practices for CASL VUQ Analysis Using Dakota

Brian M. Adams (SNL), Russell W. Hooper (SNL), Ralph C. Smith (NCSU), Brian J. Williams (LANL)

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

# Outline

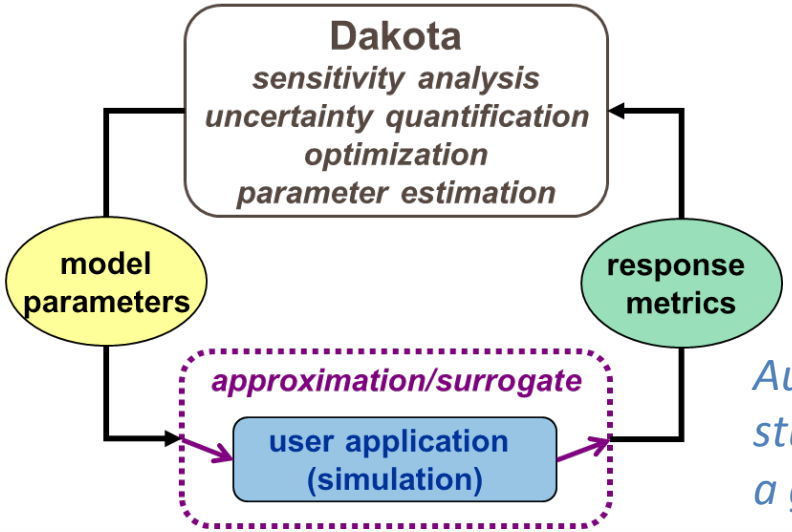
- Overview of Dakota
  - Dakota is part of VERA
- Goals of CASL Dakota Manual
  - Support code and application PCMM
- Overview of Cobra-TF Application
  - Input parameter exposure in Cobra-TF
- Overview of VUQ methods covered
  - Sensitivity analysis, optimization and deterministic calibration, mathematical surrogate construction, UQ, Bayesian model calibration
- Cobra-TF Application
  - Solution verification, sensitivity analysis, kriging surrogate construction, Bayesian model calibration
- Conclusions

CASL Dakota manual facilitates VUQ analysis via worked applications

# Dakota Supports Simulation Credibility

- Provides broader and deeper perspective for analysts and decision makers
  - *Enhances understanding of risk by quantifying margins and uncertainties (QMU)*
  - *Improves products through simulation-based design*
  - *Assesses simulation credibility through verification and validation*
- Enables QMU and design with simulations in manner analogous to experiment-based QMU and physical design/test cycles

Manages and analyzes ensembles of simulations:



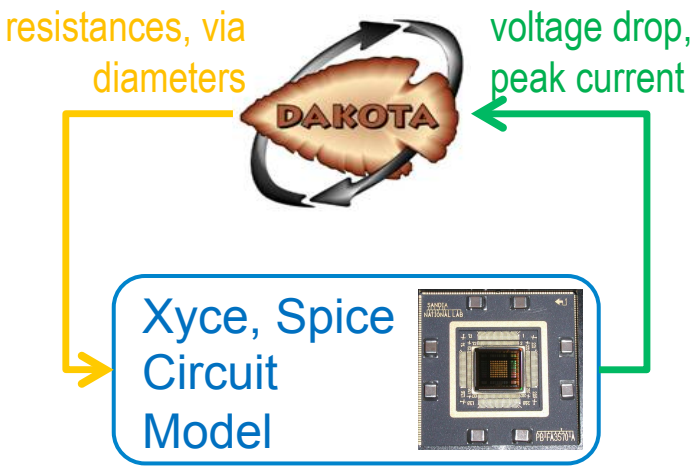

*Automate typical "parameter variation" studies with various advanced methods and a generic interface to your simulation.*

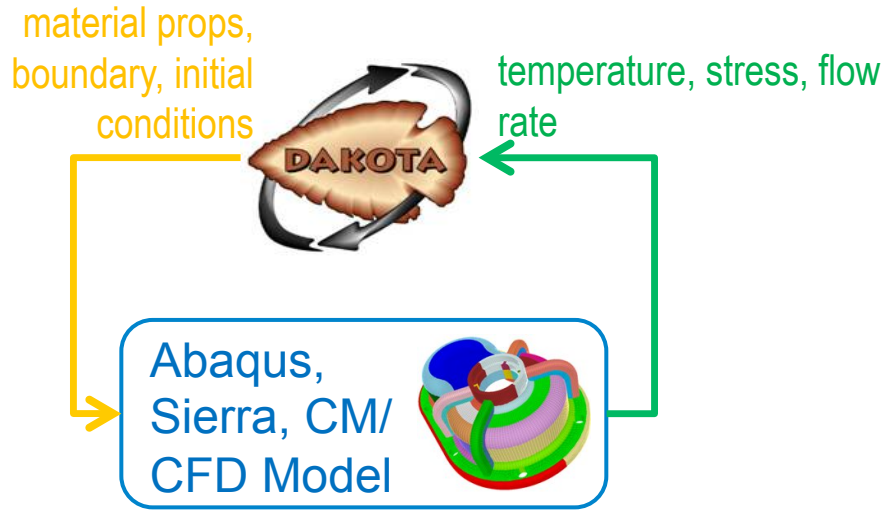
**Dakota tailors code iterations to efficiently solve VUQ problems**

# Advanced Exploration of Simulations

**Dakota enriches simulations to address analyst/designer questions:**

- Which are crucial factors/parameters, how do they affect key metrics? *(sensitivity)*
- How safe, reliable, robust, or variable is my system?
  *(quantification of margins and uncertainty: QMU, UQ)*
- What is the best performing design or control? *(optimization)*
- What models and parameters best match experimental data? *(calibration)*



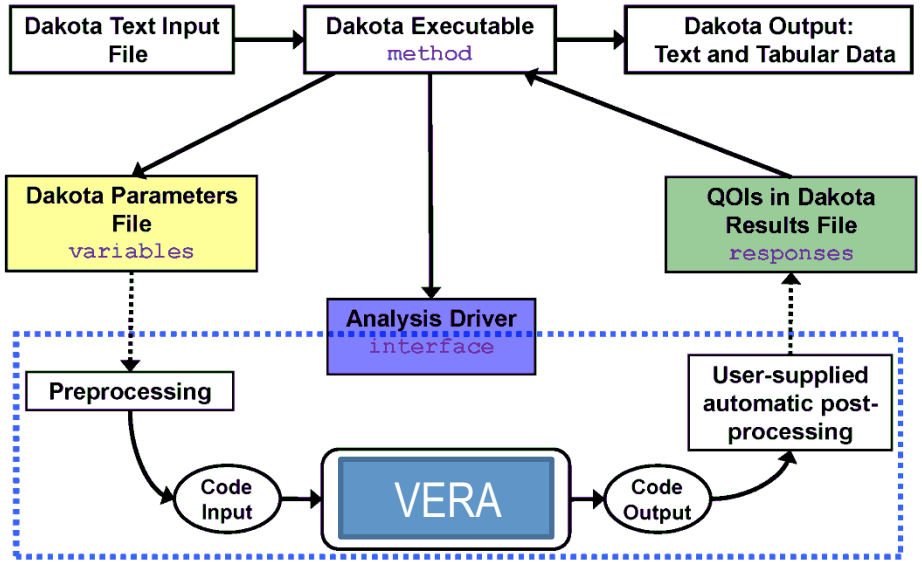

*All based on iterative analysis of a computational model for phenomena of interest*

- Commercial or SNL, loose-coupled/black-box or embedded/tightly integrated…

**Dakota supports multiple interfaces for code interactions**

# Dakota Status in VERA

- Dakota synced from SNL to CASL and builds/tests in VERA to protect integration investment
- Examples in `VUQDemos` archive previous studies and test against development physics code inputs
- Focusing on loose, but validating workflows since there isn't a single coupled physics driver in VERA
- *Accumulating technical debt due to challenges adapting Dakota to VERA build infrastructure*




- Manipulate parameters in:
  - VERA Input
  - VUQ auxiliary data, e.g., model form
  - Offline generated input data such as meshes or cross sections
- Work in progress for better QOI extraction

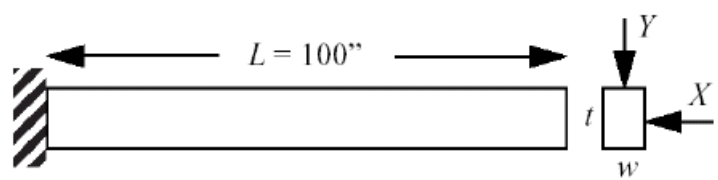
**Dakota enables core VUQ analyses in CASL**

# Manual Includes Dakota Basics

- Dakota's relationship to PCMM
- Why use Dakota: key capabilities
- How to access the software, help resources, and examples
- Interacting with Dakota, at a high level
- How Dakota input files and simulation interfaces work
- *Not exhaustive: defers to core Dakota manuals for details!*
- Accessible cantilever beam example with simplified governing equations

Table 1.1: Summary of Dakota relevance for PCMM-related activities.

| VUQ/PCMM Activity | Dakota relevance |
|---|---|
| select quantities of interest (QOIs) | (limited) |
| software quality assurance (SQA) | (limited) |
| code verification | conduct parameter studies as a function of mesh quality; calculate convergence rate |
| solution verification | conduct parameter studies over solver parameters or mesh quality; calculate convergence rate |
| validation | run ensemble of simulations and make (potentially uncertainty-aware) comparisons with experimental data, assess model form uncertainty |
| sensitivity | conduct global sensitivity analysis to rank or screen parameters; supports quantified parameter ranking table (QPRT) |
| uncertainty quantification | compute uncertainty in QOIs for risk-informed decision making |
| calibration | tune or refine models for use in particular scenarios |




$$\texttt{area} = wt$$

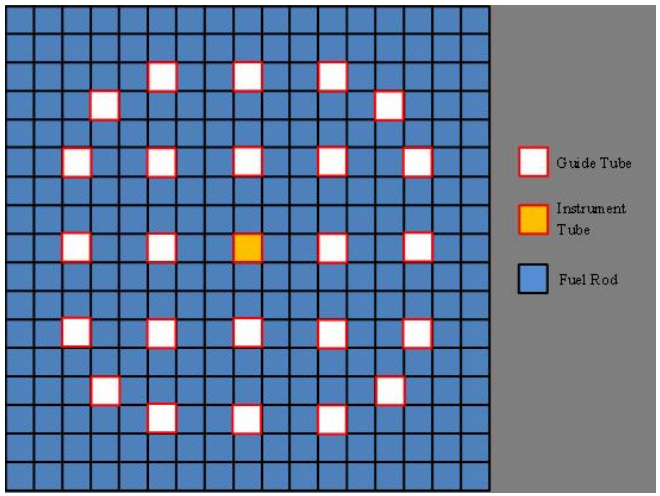
$$\texttt{stress} = S - R = \frac{600}{wt^2}Y + \frac{600}{w^2t}X - R$$

$$\texttt{displacement} = D - D_0 = \frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} - D_0$$

**Dakota enhances code and application PCMM**

# VUQ Analysis of Cobra-TF for Progression Problem 6

- Simulation of a single PWR assembly
  - Hot Full Power, T/H feedback
  - Boron concentration of 1300 ppm, 100% power
  - Power supplied by neutronics held constant




- Two CASL VUQ workflows support Cobra-TF parameter variation
  - Dakota integration with VERA common input tool suite
  - Dakota perturbation of "VUQ parameters" associated with closure laws
- Dakota studies illustrate application of VUQ methodologies described in the manual
  - 33 "VUQ parameters" exposed to Dakota for perturbation
  - Quantity of Interest: Total pressure drop through fuel rod assembly

**Dakota studies illustrated with worked examples for Cobra-TF**



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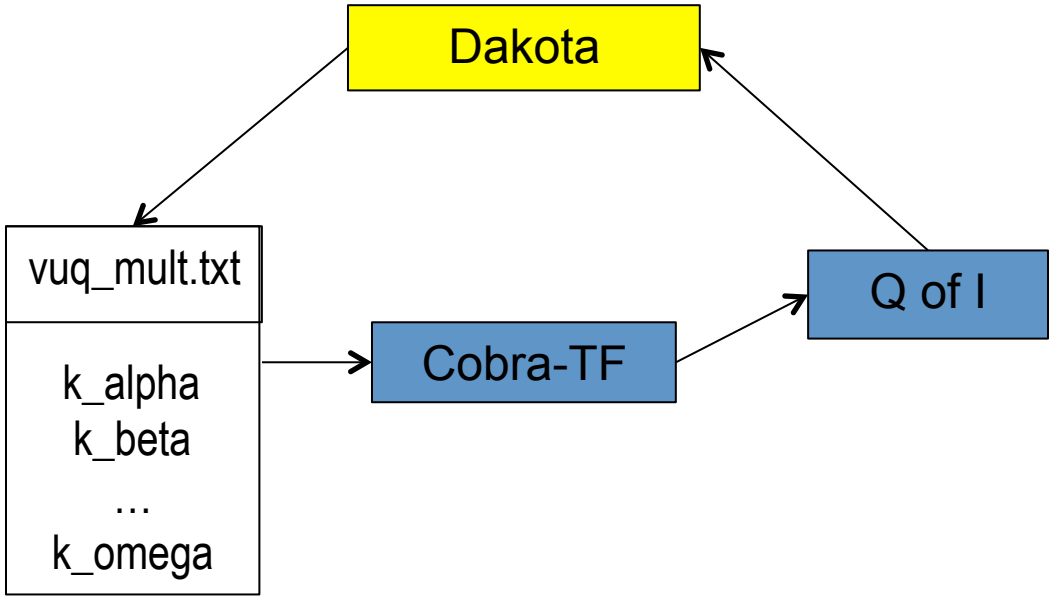
# Cobra-TF Parameter Exposure

## with Noel Belcourt

For general parameter perturbations:

$$\alpha = k_\alpha \alpha_0 + s_\alpha$$



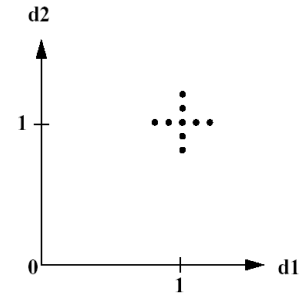

This capability enables:

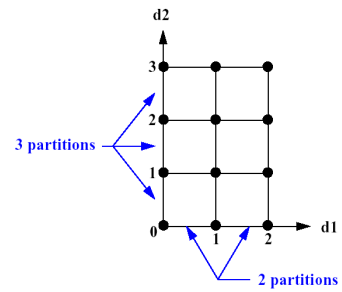
- Sensitivity studies
- Uncertainty Quantification studies
- Parameter optimization and calibration

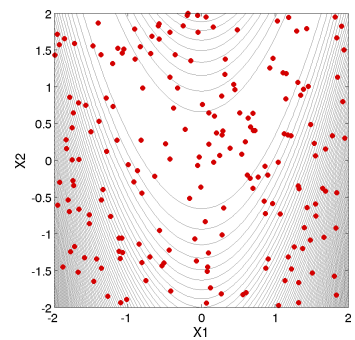
**Exposure of CTF input parameters enables VUQ analysis**

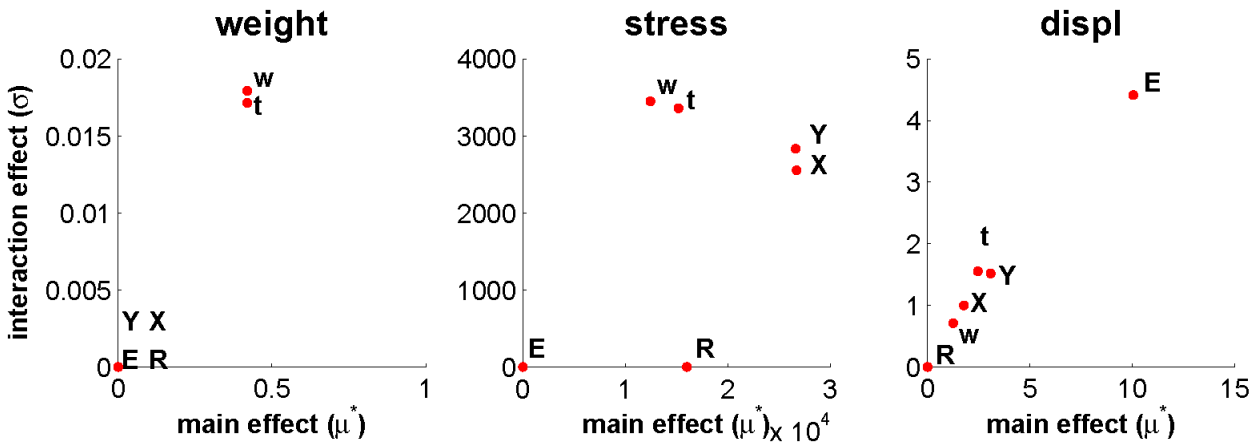
# Dakota Sensitivity Analysis

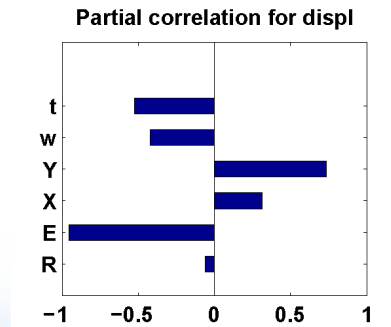
- Overview of sensitivity analysis goals, terminology, and metrics
- Details on basic centered and tensor grid parameter studies; analysts typically conduct them anyway
- Emphasized global Latin hypercube sampling and Morris designs:
  - Sample paths around global space in coordinate directions
  - Give good measure of main (linear, first-order) and interaction / nonlinear effects for modest simulation budget




**Dakota facilitates discovery of input parameter effects**

# Dakota Optimization and Calibration

- Survey of optimization goals and problem formulations, including considerations for calibration to experimental data
- Emphasized one each gradient-based, derivative-free local, and global algorithm and how to select from among them

$$
\begin{aligned}
\texttt{minimize} \quad & \texttt{area} = wt \\
\texttt{subject to} \quad & \texttt{stress} = S - R \leq 0 \\
& \texttt{displacement} = D - D_0 \leq 0 \\
& 1.0 \leq w \leq 4.0 \\
& 1.0 \leq t \leq 4.0
\end{aligned}
$$

```
<<<<< Function evaluation summary: 18 total (18 new, 0 duplicate)
<<<<< Best parameters          =
                     2.4000000000e+00 w
                     3.5000000000e+00 t
                     4.0000000000e+04 R
                     2.9000000000e+07 E
                     5.0000000000e+02 X
                     1.0000000000e+03 Y
<<<<< Best objective function  =
                     8.4000000000e+00
<<<<< Best constraint values   =
                    -4.7108843537e+03
                    -2.9685051703e-01
```

Table 5.1: Guidance for selecting from the top recommended Dakota optimization algorithms.

| algorithm type / Dakota method | variable type | cost (samples) | goal and characteristics |
|---|---|---|---|
| gradient-based local/ OPT++ Quasi-Newton | continuous | low/ medium | single local solution/improvement, assumes smooth input/output mapping |
| *local calibration* / OPT++ Gauss Newton | continuous | low/ medium | same as previous line, but tailored to least-squares calibration |
| derivative-free local / Coliny Pattern Search | continuous | medium/ high | single local solution; better when can't estimate derivatives |
| *local w/surrogate* / Surrogate-based Local | continuous | medium | same as "derivative-free local," but for noisier or more expensive simulations |
| global / Coliny Evolutionary Algorithm | continuous or discrete | high | global optimality, with ranked family of best solutions |
| *global w/surrogate* / Efficient Global | continuous | medium | same as "global," but for more expensive simulations |

**Dakota offers multiple code optimization/calibration options**



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# Guidance on Navigating All Dakota Methods

- Sensitivity Analysis

Table 3.2: Guidelines for selection of parameter study, DOE, DACE, and sampling methods.

| Method Classification | Applications | Applicable Methods |
|---|---|---|
| parameter study | sensitivity analysis, directed parameter space investigations | centered_parameter_study, list_parameter_study, multidim_parameter_study, vector_parameter_study |
| classical design of experiments | physical experiments (parameters uniformly distributed) | dace (box_behnken, central_composite) |
| design of computer experiments | variance analysis, space filling designs (parameters uniformly distributed) | dace (grid, random, oas, lhs, oa_lhs), fsu_quasi_mc (halton, hammersley), fsu_cvt, psuade_moat |
| sampling | space filling designs (parameters have general probability distributions) | sampling (Monte Carlo, LHS) with optional active view override |

- Optimization

Table 5.2: Detailed guidelines for selecting from among all Dakota optimization methods. Blank fields inherit the values from above.

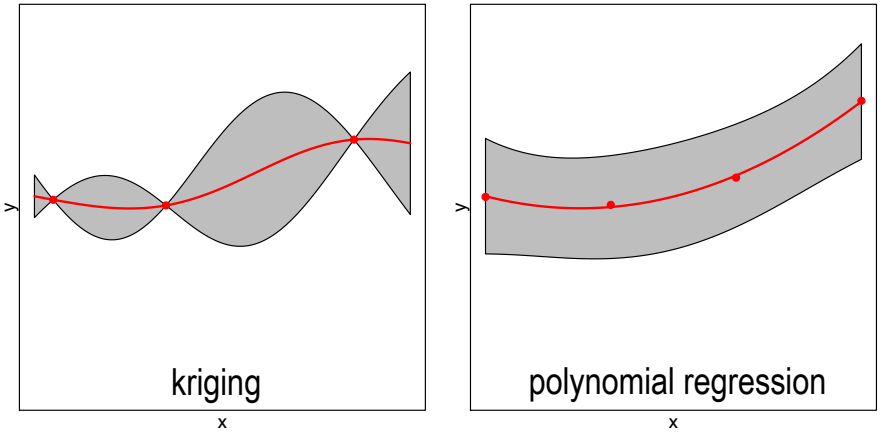
| Method Classification | Desired Problem Characteristics | Applicable Methods |
|---|---|---|
| Gradient-Based Local | smooth; continuous variables no constraints | optpp_cg |
| | smooth; continuous variables; bound constraints | dot_bfgs, dot_frcg, conmin_frcg |
| | smooth; continuous variables; bound constraints, linear and nonlinear constraints | npsol_sqp, nlpql_sqp, dot_mmfd, dot_slp, dot_sqp, conmin_mfd, optpp_newton, optpp_q_newton, optpp_fd_newton, weighted sums (multiobjective), pareto_set strategy (multiobjective) |
| Gradient-Based Global | smooth; continuous variables; bound constraints, linear and nonlinear constraints | hybrid_strategy, multi_start strategy |
| Derivative-Free Local | nonsmooth; continuous variables; bound constraints | optpp_pds |
| | nonsmooth; continuous variables; bound constraints, linear and nonlinear constraints | asynch_pattern_search, coliny_cobyla, coliny_pattern_search, coliny_solis_wets, surrogate_based_local |
| | nonsmooth; continuous variables; discrete variables; bound constraints, nonlinear constraints | mesh_adaptive_search |
| Derivative-Free Global | nonsmooth; continuous variables; bound constraints | ncsu_direct |
| | nonsmooth; continuous variables; bound constraints, linear and nonlinear constraints | coliny_direct, efficient_global, surrogate_based_global |
| | nonsmooth; continuous variables, discrete variables; bound constraints, linear and nonlinear constraints | coliny_ea, soga, moga (multiobjective) |

**Explicit recommendations provided for choosing covered methods**

# Mathematical Surrogate Construction

**Steps:**

1. Run a simulation experiment to collect figures of merit at designed input parameter locations.
2. Fit polynomial or kriging surrogate model to experiment results and utilize in follow-on analyses.




**Motivation:**

- Enables VUQ analyses when code calculations are time consuming and no computationally efficient physics-based surrogate is readily available.

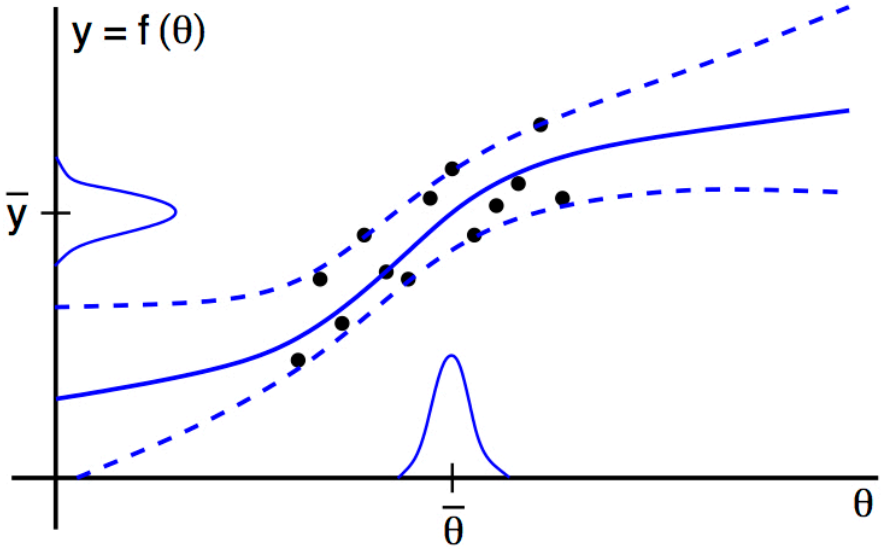
| Method | Desired Problem Characteristics | Routines |
|---|---|---|
| Polynomial regression | Smooth fit to physical experiment or stochastic/noisy code response | polynomial <trend> |
| Kriging | Interpolation of deterministic smooth code response or smooth fit to stochastic/noisy code response | gaussian_process surfpack trend <option> nugget <value> find_nugget |

Surrogate model motivation and process

# Uncertainty Quantification

**Steps:**

1. Quantify input uncertainties associated with parameters, initial and boundary conditions, or exogenous forces.
2. Propagate input uncertainties through models to construct prediction interval for quantity of interest.




**Motivation:**

- Facilitate optimal design and decision making, ensure robustness, performance or safety margins.
- E.g., outputs for emergency core cooling systems include peak cladding temperatures, maximum local cladding oxidation.

Uncertainty quantification motivation and process

# Uncertainty Propagation in Dakota

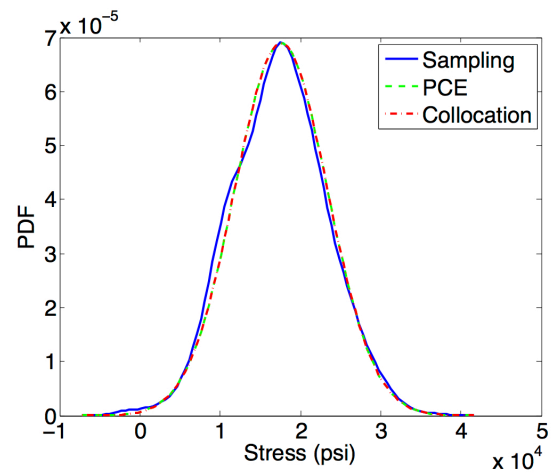
| Method | Desired Problem Characteristics | Routines |
|---|---|---|
| Sampling | Nonsmooth and/or multi-modal response functions; general densities; computationally efficient models or surrogates | sampling |
| Stochastic Polynomial | Smooth response functions; can be combined with Dakota sparse grid routines | polynomial_chaos<br>stoch_collocation |

**Representation:**

$$Y(X) = \sum_{j=0}^{J} \alpha_j \Psi_j(X)$$

**Example:** Cantilever beam – Normally distributed input parameters, stress response

| | Mean | Std. Dev. | Skewness | Kurtosis |
|---|---|---|---|---|
| Analytic | 1.760e+04 | 5.787e+03 | --- | --- |
| Sampling | 1.735e+04 | 5.809e+03 | -6.505e-03 | 7.352e-02 |
| PCE | 1.760e+04 | 5.787e+03 | 9.410e-15 | 6.271e-15 |
| Collocation | 1.760e+04 | 5.787e+03 | -1.842e-14 | 5.773e-15 |




Multiple methods used to verify Dakota propagation routines

# Bayesian Model Calibration

**Bayes' Relation:**

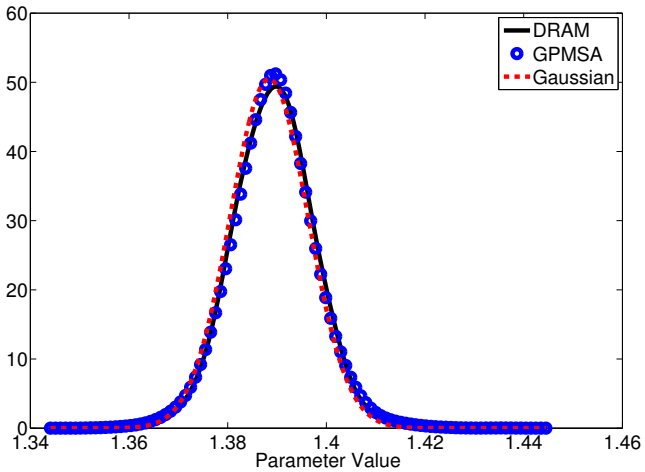
$$\pi(\theta|d) = \frac{\mathcal{L}(\theta;d)\pi_0(\theta)}{\int_{\Re^M} \mathcal{L}(\theta;d)\pi_0(\theta)d\theta}$$

Likelihood: Incorporates model and data

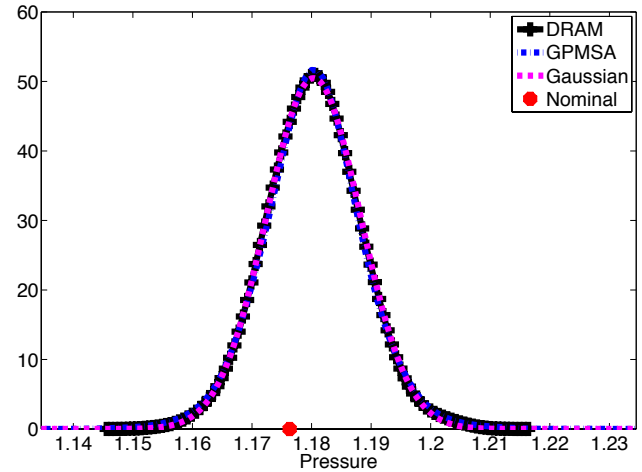
$$\mathcal{L}(\theta;d) \prod_{i=1}^{N} \frac{1}{\sigma\sqrt{2\pi}} e^{-(d_i - y_i(\theta))^2/2\sigma^2}$$

| Method | Problem Characteristics |
|---|---|
| DRAM | Well-behaved posterior densities; computationally efficient models or surrogates |
| DREAM | Complex posteriors; inherently parallel codes |
| GPMSA | Employs Gaussian process emulator; can accommodate certain model discrepancies |

**Example:** COBRA-TF parameters k_tmasl, k_tmoml, k_tnrgl, k_xkwlx, k_cd




$$\eta = 0.906\,\texttt{k_xkwlx} + 0.478\,\texttt{k_cd}$$




Output UQ via GP surrogate with inputs from DRAM chain

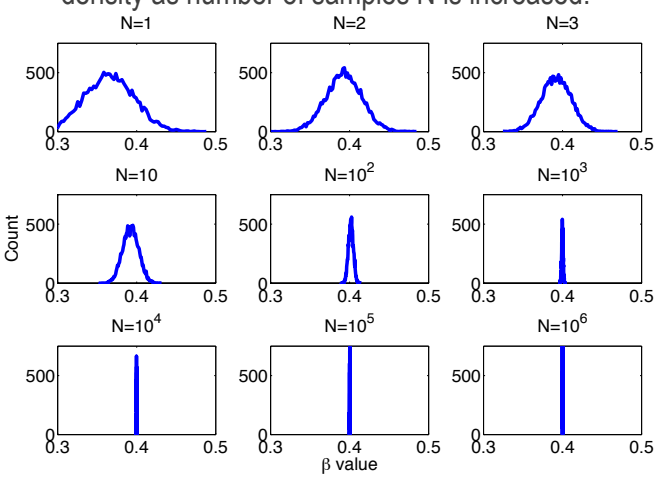
**Parameter uncertainty quantified by experimental data**

# Linear Verification Test Suite

**Objective:**

- Provide hierarchy of models to test convergence of Bayesian model calibration algorithms through comparison with analytic solutions;
- Provide regime to test accuracy of uncertainty propagation algorithms since one can employ analytic relations between input and output densities;
- Facilitate the testing of algorithms for heavy-tailed distributions;
- Provide framework for analytically testing algorithms to construct Sobol global sensitivity indices.

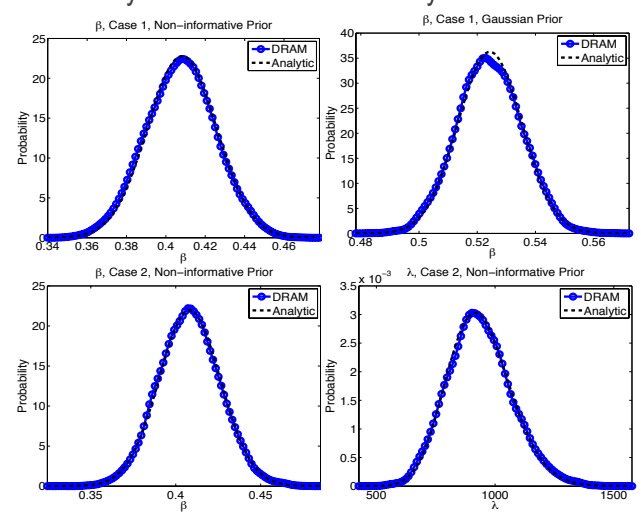
**Example:** Histograms of β converging to Dirac density as number of samples N is increased.




**Linear Regression Model:**

$$Y = G\beta + \varepsilon(\lambda, \phi)$$

**Example:** PDF estimates of β and λ from Bayesian calibration vs. analytical solutions.




"Code"/solution verification of Bayesian calibration methods

# Cobra-TF Solution Verification

## Progression Problem 6 CTF-only

- Initial study produced very good agreement with theoretical expectation (b=0.946 compared to 1.0)
- Problem 6 involves spacer grids of unequal spacing (top & bottom different than interior) requiring meshes characterized by multiple $\Delta z$ values
- Attempts to lump these into a singe $\Delta z$ produced poor orders-of-convergence, eg ~0.7 (see report)
- A sensitivity study of total pressure drop on spacer grid locations showed low sensitivity, < 0.2%
- Spacer grid locations were shifted to produce meshes characterized by a single $\Delta z$, and the solution verification study was repeated

**Axial mesh refinement convergence studies for CTF**



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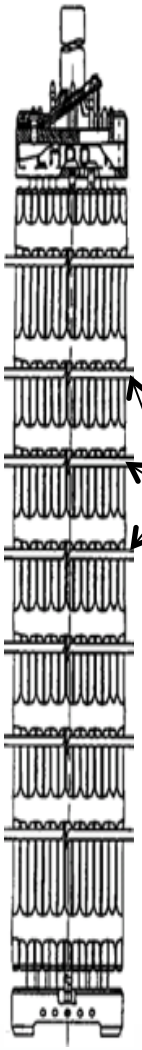
# Cobra-TF Solution Verification

## Progression Problem 6 CTF-only: No Spacer Grids



Omit Spacer Grids

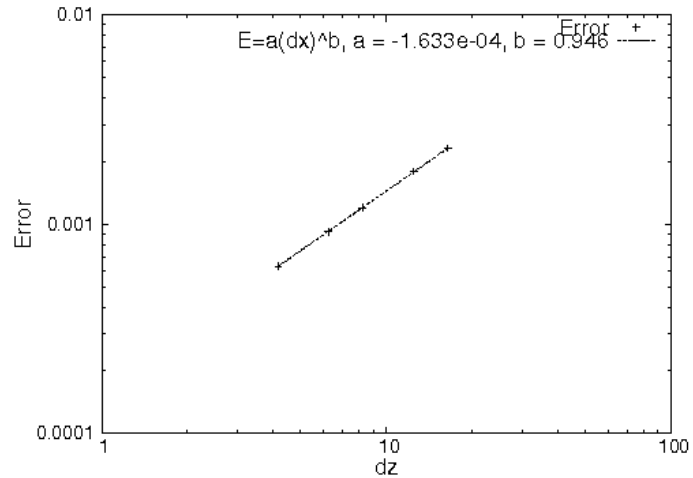
| CTF-only Problem 6, No Grids | | | |
|---|---|---|---|
| Mesh factor, f | Δz (cm) | #Axial elements | Tot. Press. (bar) |
| 0.5 | 4.160 | 87 | 0.68788 |
| 0.75 | 6.240 | 58 | 0.68759 |
| 1.0 | 8.225 | 44 | 0.68731 |
| 1.5 | 12.479 | 29 | 0.68673 |
| 2.0 | 16.450 | 22 | 0.68620 |

Error Model:

$$P = \bar{P} + a\,(\Delta z)^b$$

$$E = P - \bar{P} = a\,(\Delta z)^b$$

$$b = 0.946$$

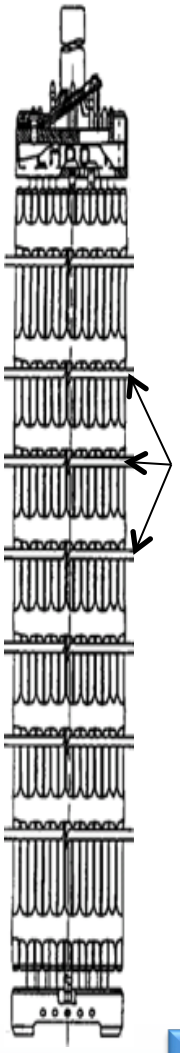



Good agreement with theoretical 1.0

**Estimated and theoretical rates consistent: no spacer grids**

# Cobra-TF Solution Verification

## Progression Problem 6 CTF-only: With Spacer Grids*



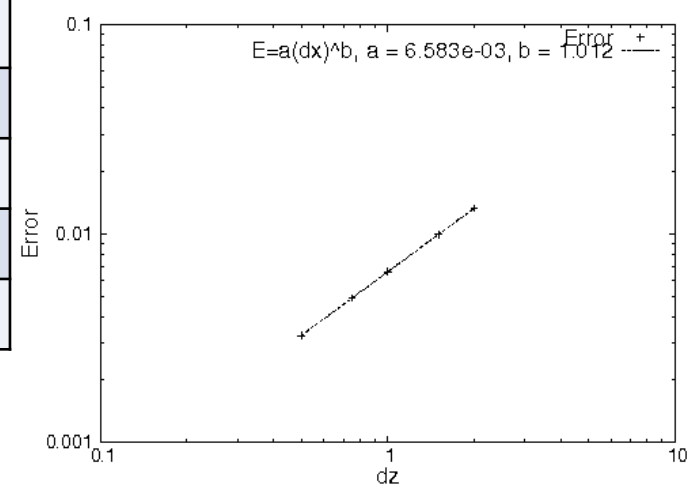

| CTF-only Problem 6, With Grids* | | | |
|---|---|---|---|
| Mesh factor, f | Δz (cm) | #Axial elements | Tot. Press. (bar) |
| 0.5 | 4.036 | 72 | 1.16843 |
| 0.75 | 6.054 | 48 | 1.1701 |
| 1.0 | 8.072 | 36 | 1.17176 |
| 1.5 | 12.108 | 24 | 1.17508 |
| 2.0 | 16.144 | 18 | 1.17845 |

* Grid locations were shifted to produce equal mesh spacing between all grids.

Error Model:

$$E = P - \bar{P} = a\,(\Delta z)^b$$

$$b = 1.012$$




Good agreement with theoretical 1.0

**Estimated and theoretical rates consistent with spacer grids**

# Cobra-TF Sensitivity Analysis

| parameter | partial correlation | simple correlation | morris main | morris interaction | CPS variation |
|---|---|---|---|---|---|
| k_eta | 0.07 | 0.03 | | | |
| k_gama | -0.03 | 0.04 | | | |
| k_sent | -0.03 | -0.02 | | | |
| k_sdent | -0.07 | -0.01 | | | |
| k_tmasv | -0.03 | 0.00 | | | |
| k_tmasl | 0.11 | 0.00 | 6.48E-05 | 2.28E-05 | medium |
| k_tmasg | -0.19 | -0.01 | | | |
| k_tmomv | -0.12 | -0.01 | | | |
| k_tmome | 0.02 | 0.00 | | | |
| k_tmoml | 0.02 | -0.02 | 2.23E-04 | 1.30E-04 | medium |
| k_xk | 0.08 | -0.02 | | | |
| k_xkes | -0.05 | 0.00 | | | |
| k_xkge | -0.07 | 0.01 | | | |
| k_xkl | 0.04 | -0.01 | | | |
| k_xkle | -0.03 | 0.00 | | | |
| k_xkvls | 0.11 | -0.01 | | | |
| k_xkwvw | -0.10 | 0.01 | | | |
| k_xkwlw | 0.14 | 0.01 | | | |
| k_xkwew | -0.01 | 0.03 | | | |
| k_qvapl | -0.09 | -0.01 | | | |
| k_tnrgv | -0.03 | 0.00 | | | |
| k_tnrgl | -0.01 | 0.03 | 9.00E-06 | 9.49E-06 | low |
| k_rodqq | 0.02 | -0.01 | | | |
| k_qradd | -0.02 | 0.00 | | | |
| k_qradv | -0.01 | 0.00 | | | |
| k_qliht | -0.01 | 0.00 | | | |
| k_sphts | -0.05 | 0.03 | | | |
| k_cond | -0.04 | 0.00 | | | |
| k_xkwvx | 0.03 | -0.02 | | | |
| k_xkwlx | 1.00 | 0.88 | 1.80E-01 | 7.07E-03 | high |
| k_cd | 1.00 | 0.46 | 9.59E-02 | 7.88E-03 | high |
| k_cdfb | -0.02 | -0.01 | | | |
| k_wkr | 0.02 | 0.02 | | | |

## 5 Active Inputs:

`k_cd` : Pressure loss coefficient of spacer in sub-channel

`k_xkwlx` : Vertical liquid wall drag coefficient

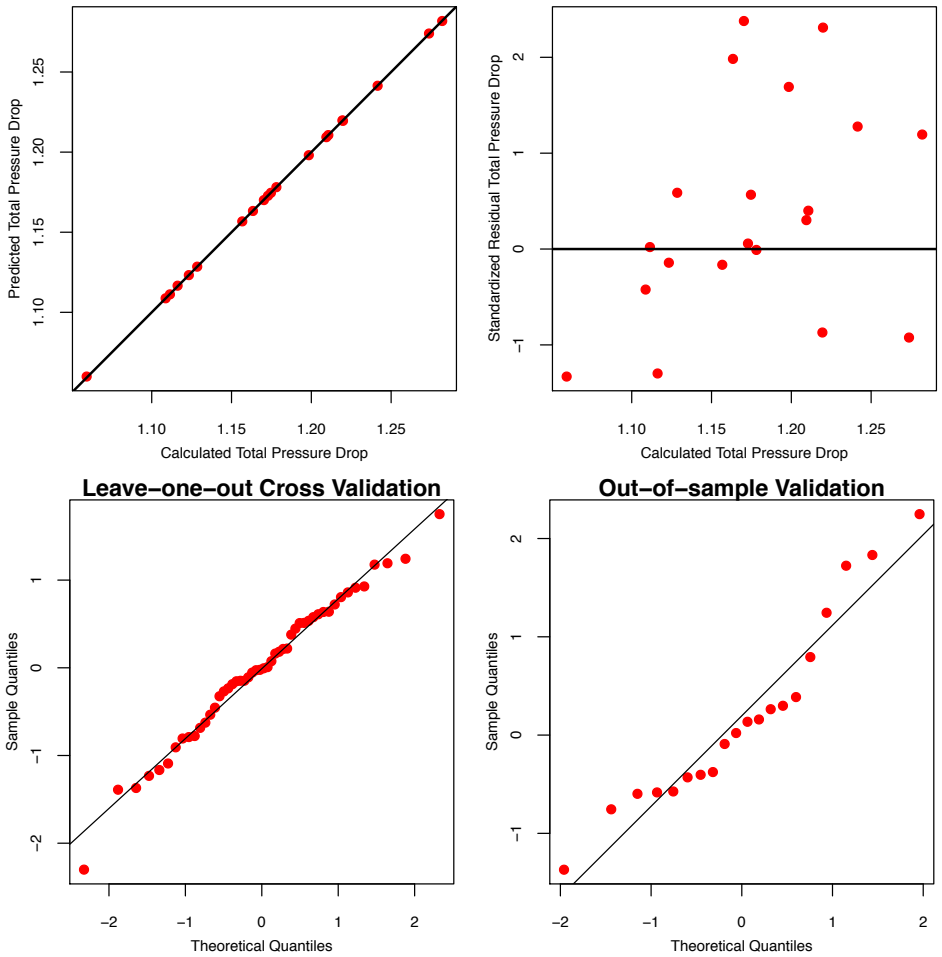
`k_tmasl` : Loss of liquid mass due to mixing and void drift

`k_tmoml` : Loss of liquid momentum due to mixing and void drift

`k_tnrgl` : Loss of liquid enthalpy due to mixing and void drift

33 initial VUQ parameters reduced to 5 via sensitivity analysis

# Cobra-TF Mathematical Surrogate Construction




Kriging surrogate for total pressure drop using 50 Cobra-TF runs perturbing 5 active inputs

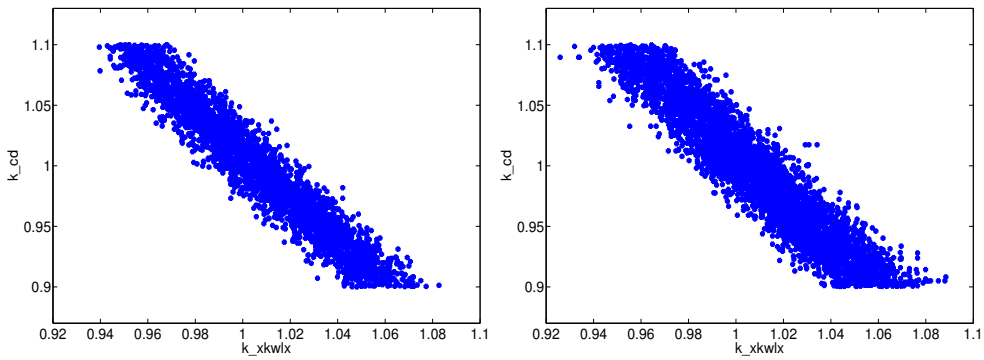
Examine the quality of surrogate fits via diagnostics post-processed from Dakota output

LOO CV RMSPE: 3.24E-4 (0.15% of observed range in pressure drop)

Validation ($N_V$ = 20) RMSPE: 2.51E-4 (0.11% of observed range in pressure drop)

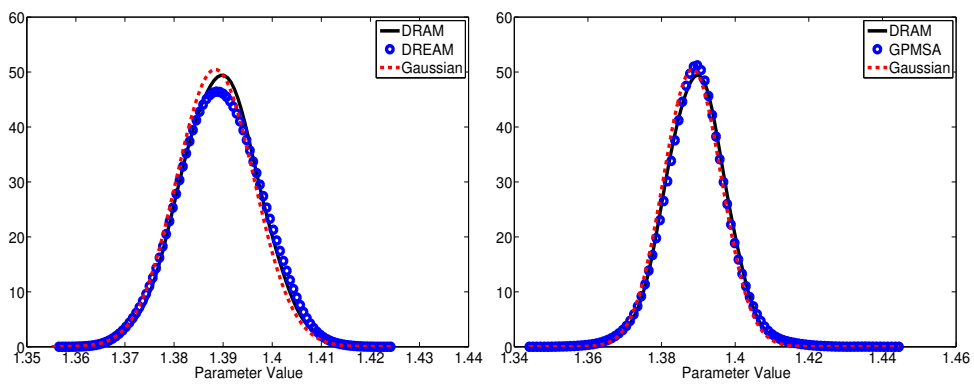
**Mathematical surrogates are used for fast computation**

# Cobra-TF Model Calibration




Synthetic experimental data generated by adding Gaussian noise to Cobra-TF total pressure drop value at nominal parameter setting.

Calibrated parameter samples from two calibration methods (DREAM, GPMSA) for `k_xkwlx` vs. `k_cd`.




$$\eta = 0.906\,\mathtt{k_xkwlx} + 0.478\,\mathtt{k_cd}$$

Verification of three Bayesian model calibration methods (DRAM, DREAM, GPMSA) applied to kriging surrogate for Cobra-TF total pressure drop. Calibrated parameter $\eta$ is approximately analytically Gaussian.

**Model calibration results in input parameter UQ consistent with data**

# Conclusions

- Manual provides an overview of core VUQ methods expected to receive heavy use in CASL applications
- Manual provides representative Dakota input decks for the core VUQ methods with worked examples of their deployment
- Manual provides references to other Dakota manuals having more extensive discussions of methods and deployment
- Manual began development of more extensive “stochastic verification” test suite to verify performance of Bayesian model calibration methods
- Collaboration on this manual has revealed the need for targeted Dakota development projects, particularly in the areas of Bayesian model calibration and interfacing reduced order modeling techniques
- Code/solution verification methods (e.g. RMR) and validation metric computation through Percept are/will be integrated into Dakota

**Continued Dakota development supports CASL-relevant VUQ analysis**