



*Exceptional
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in the
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interest*

Dakota Software Training

Uncertainty Quantification

<http://dakota.sandia.gov>



U.S. DEPARTMENT OF
ENERGY



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Module Learning Goals

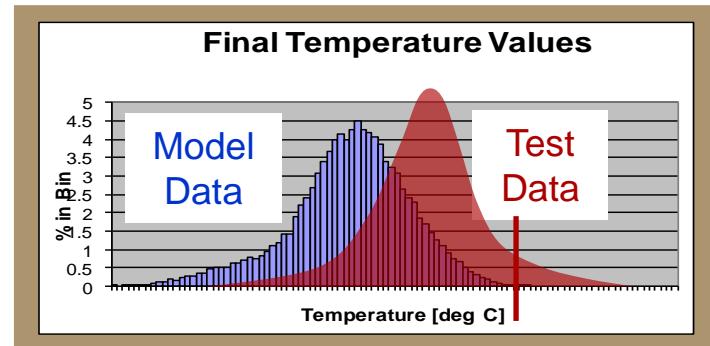
- Understand why you might want to perform uncertainty quantification (UQ)
- Understand prerequisites and have a practical process for UQ at your disposal
- Be able to formulate your problem, present it to Dakota, and run and understand studies
- Be able to select an appropriate Dakota UQ method
- Know how to use Dakota UQ results

Module Outline

- Introduction: application examples to define UQ, illustrate the UQ process, and explain why you might care
- UQ terminology: characterizing and expressing your problem to Dakota
- Monte Carlo sampling for UQ
- **Exercise: Dakota input and output for Monte Carlo sampling**
- Selecting an uncertainty quantification method; reliability and polynomial chaos
- **Exercise: Comparing UQ methods and problem assumptions**
- Beyond Dakota: follow-on activities using UQ results
- Summary of advanced topics and references

Why Uncertainty Quantification?

- **What?** Determine variability, distributions, statistics of code outputs, given uncertainty in input factors; *put error bars on simulation output*
- **Why?** Tactically, assess likelihood of typical or extreme outcomes. Given input uncertainty...
 - Determine mean or median performance of a system
 - Assess variability or robustness of model response
 - Find probability of reaching failure/success criteria (reliability metrics)
 - Assess range/intervals of possible outcomes
- Ultimately, use simulations for risk-informed decision making, e.g., assess how close uncertainty-endowed code predictions are to
 - Experimental data
(validation, is model sufficient for the intended application?)
 - Performance expectations or limits
(quantification of margins and uncertainties; QMU)

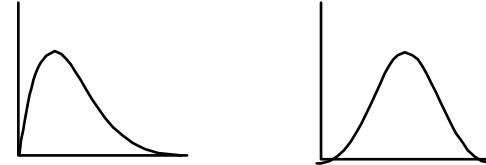
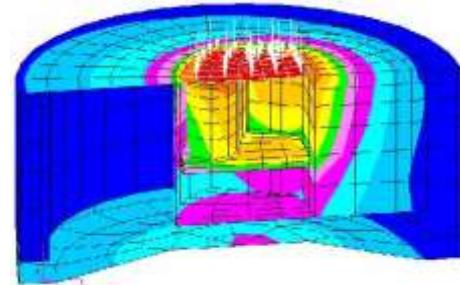


Example:

Thermal Uncertainty Quantification

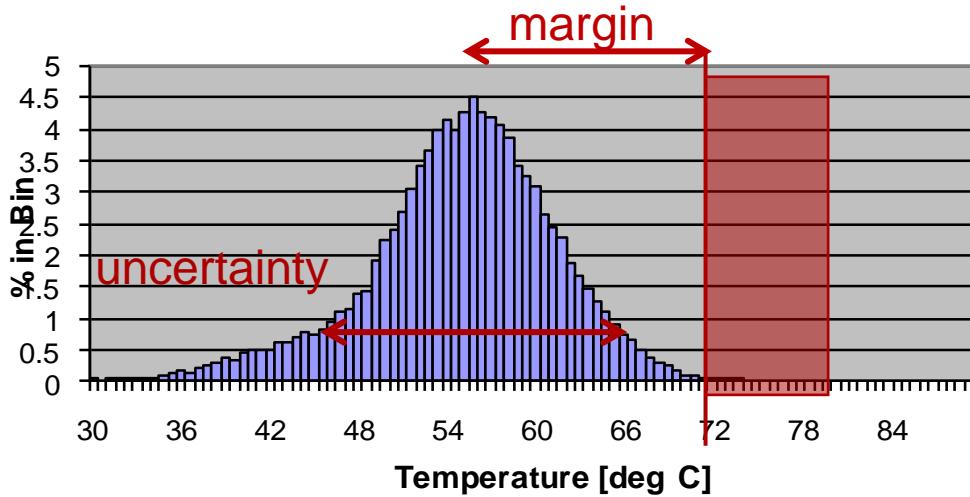


- Device subject to heating (experiment or corresponding computational simulation)
- Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by u_1, \dots, u_N
- Response temperature $f(u) = T(u_1, \dots, u_N)$ calculated by heat transfer code



Given distributions of u_1, \dots, u_N , UQ methods calculate statistical info on outputs:

Final Temperature Values



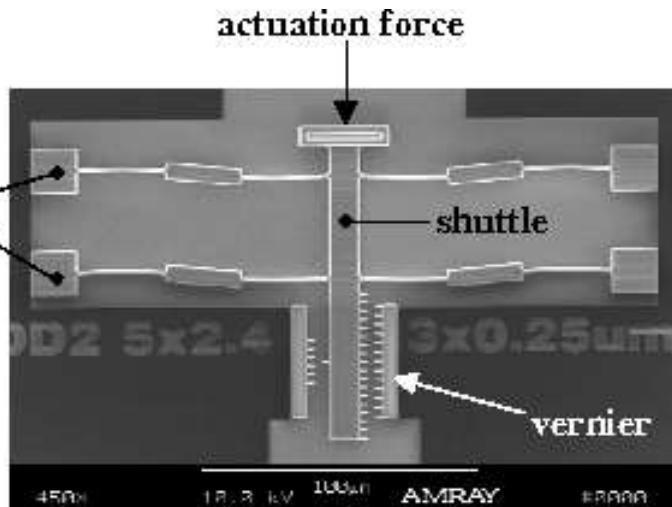
- Mean(T), standard deviation(T), Probability($T \geq T_{\text{critical}}$)
- Probability distribution of temperatures
- Bounds on temperature (min/max)

Example:

MEMS Manufacturing Uncertainty



- **Micro-electromechanical system (MEMS):** typically made from silicon, polymers, or metals; used as micro-scale sensors, actuators, switches, and machines
- **MEMS designs:** subject to substantial variability, lack historical knowledge base; uncertainty from materials, micromachining, photo lithography, etching process
- Resulting part yields can be low or have poor cycle durability
- **Goal:** UQ with finite element model of bi-stable switch to...
 - Assess reliability in predicted actuation force and variability in min/max force
 - Minimize sensitivity to uncertainties (robustness)



*uncertain parameters:
edge bias and residual stress*

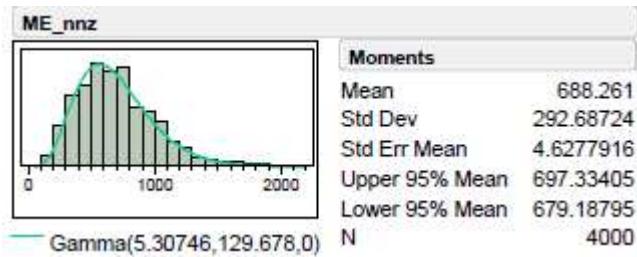
variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

Example: Uncertainty in Boiling Rate in Nuclear Reactor Core (DOE CASL)

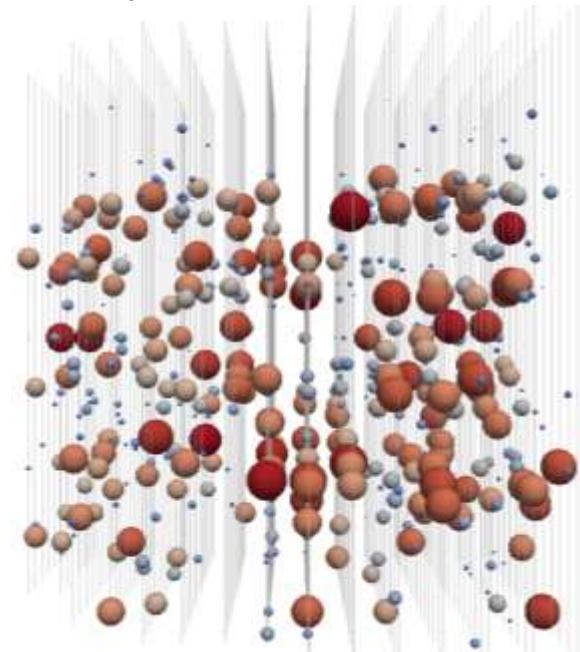
- Use nuclear reactor thermal-hydraulics model to **assess uncertainty in localized boiling due to variable operating conditions**
- Compare Dakota UQ approaches and modelling assumptions

Method	ME_nnzs		ME_meannnzs		ME_max	
	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
LHS (40)	651.225	297.039	127.836	27.723	361.204	55.862
LHS (400)	647.33	286.146	127.796	25.779	361.581	51.874
LHS (4000)	688.261	292.687	129.175	25.450	364.317	50.884
PCE ($\Theta(2)$)	687.875	288.140	129.151	25.7015	364.366	50.315
PCE ($\Theta(3)$)	688.083	292.974	129.231	25.3989	364.310	50.869
PCE ($\Theta(4)$)	688.099	292.808	129.213	25.4491	364.313	50.872

mean and standard deviation of key metrics



normally distributed inputs need not give rise to normally distributed outputs...



anisotropic uncertainty distribution in boiling rate throughout quarter core model (side view)

Discussion:

Uncertainties in Your Domain



- What are the key uncertainties that affect your experiments, analysis, and work products?
- How do you account for them when using science and engineering computational models?

A Practical Process for UQ

1. Determine your UQ analysis goal
 - What are the key model responses (quantities of interest)
 - What kinds of statistics or metrics do you want on them?
2. Identify potentially influential uncertain input parameters
 - Includes parameters that influence trend in response as well as those that influence variability in response
3. Characterize input uncertainties and map them into Dakota variable specifications
4. What are the model characteristics/behaviors? Recall:
 - Simulation cost, model robustness, input/output properties such as kinks, discontinuities, multi-modal, noise, disparate regimes*covered in other modules*
5. Select a method appropriate to variables, goal, and problem
6. Set up Dakota input file and interface to simulation
7. Run study and interpret the results

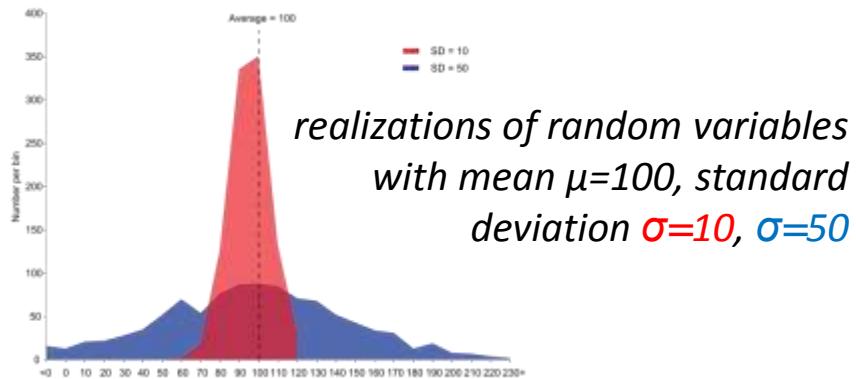
Up next: Discuss 1, 2 and 3, relate to Dakota, and see a simple example of 6, 7

Familiarize Yourself with Key Statistics Ideas: Moments of Random Variables

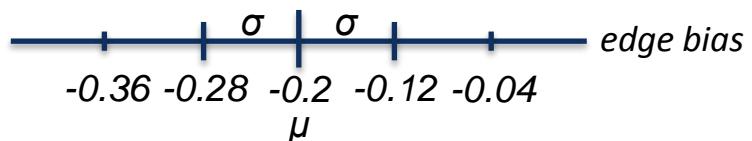
Understanding the following basic concepts will help with Dakota UQ

- Concept of a random variable X
- Mean (m, μ): expected or average value of X , e.g., *mean of sample of size N* :
$$\mu_T = \frac{1}{N} \sum_{i=1}^N T(u^i)$$
- Standard deviation (s, σ): measure of dispersion / variability of X :

$$\sigma_T = \sqrt{\frac{1}{N} \sum_{i=1}^N [T(u^i) - \mu_T]^2}$$



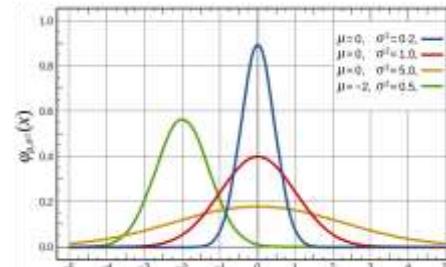
In the earlier MEMS application, the manufactured edge has a mean bias of $-0.2 \mu\text{m}$, with standard deviation $0.08 \mu\text{m}$:



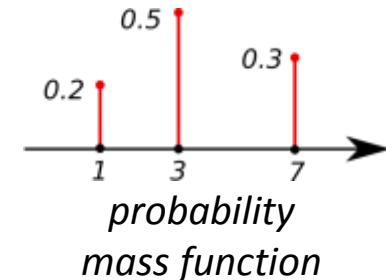
Familiarize Yourself with Key Statistics Ideas: PDFs, CDFs, Intervals

Understanding the following basic concepts will help with Dakota UQ

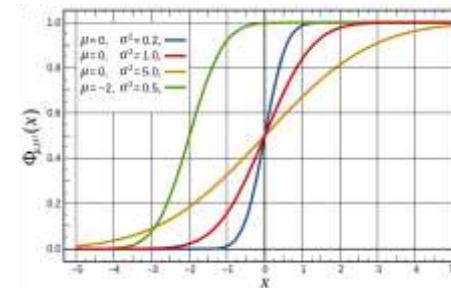
- Probability density / probability mass function: relative likelihood of a given value of X
- Cumulative distribution function: probability that X will take on a value less than or equal to x :
 $P(X \leq x)$
- Interval-valued uncertainty: X can take on any value in the interval $[a, b]$, but no probability or likelihood of one value vs. another



probability density functions



probability mass function

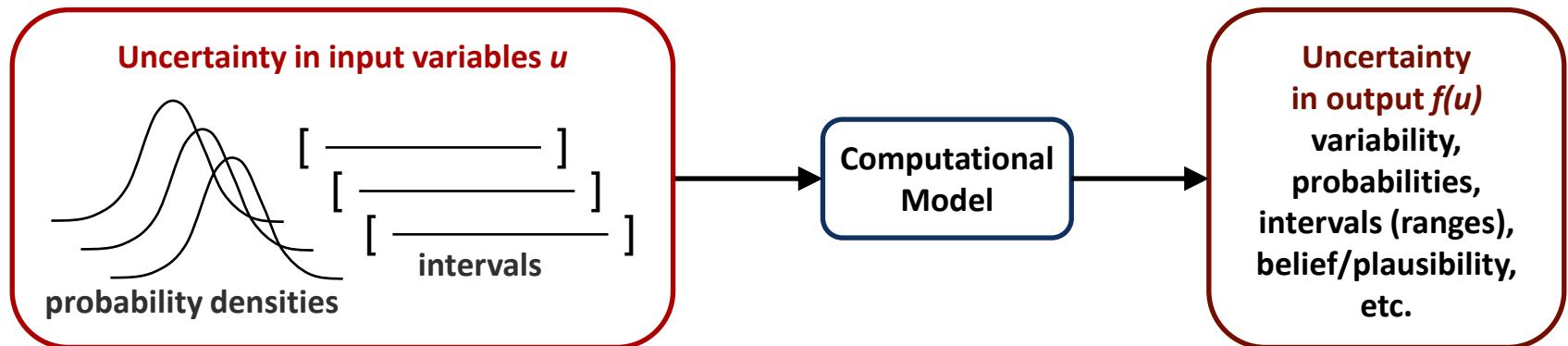


cumulative distribution functions

For the earlier thermal application, a **PDF or CDF** can answer questions about the probability of exceeding a critical temperature.

Dakota Uncertainty Quantification

- Dakota UQ methods primarily focus on **forward propagation of parametric uncertainties** through a model: *determine uncertainty in model output, given uncertainty in input parameters*

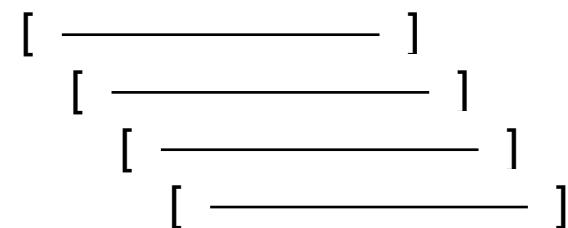
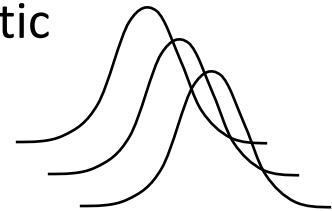


- Example uncertain inputs: physics parameters, material properties boundary/initial conditions, operating conditions, model choice, geometry
- Can also perform “inverse UQ” to determine uncertainties in parameters consistent with data (not covered in this module)*

Categories of Uncertainty

This distinction can help in selecting Dakota variable types and method

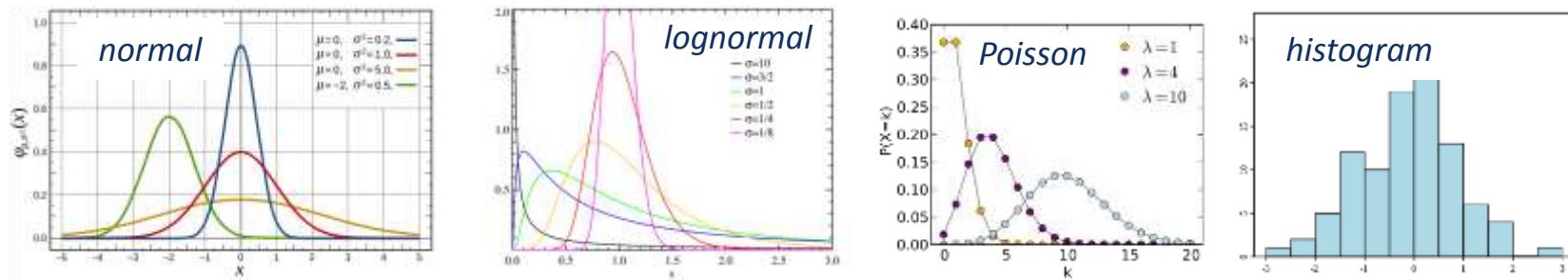
- **Aleatory** (*think probability density function, frequency; sufficient data*)
 - Inherent variability (e.g., in a population), type-A, stochastic
 - Irreducible: further knowledge won't help
 - Ideally simulation would incorporate this variability
- **Epistemic** (*e.g., bounded intervals, distribution with uncertain parameters*)
 - Subjective, type-B, state of knowledge uncertainty
 - Reducible: more data or information, would make uncertainty estimation more precise
 - Fixed value in simulation, e.g., elastic modulus, but not well known for this material



See separate course on motivation for aleatory vs. epistemic uncertainty

Characterizing Uncertainties to Dakota

- Must characterize each variable's uncertainty and (optionally) any correlation between pairs of variables. **Need not be normal (or uniform)!**
- May require processing data with math/stats tool to fit distributions, performing literature searches, or querying experts



Dakota **uncertain variable** types:

- Aleatory continuous:** normal, lognormal, uniform, loguniform, triangular, exponential, beta, gamma, Gumbel, Frechet, Weibull, histogram
- Aleatory discrete:** Poisson, binomial, negative binomial, hypergeometric, histogram point (integer, real, string)
- Epistemic:** continuous interval, discrete interval, discrete set

Specifying Dakota Uncertain Variables

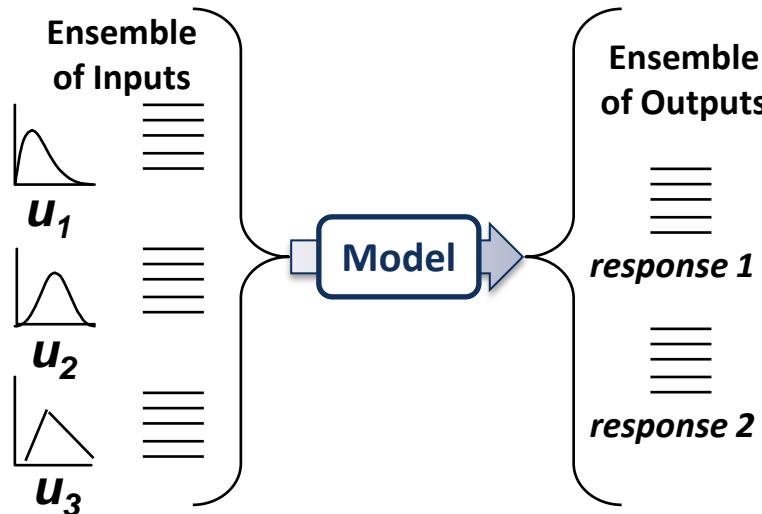
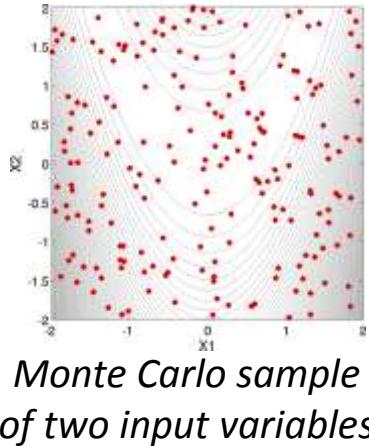
- UQ problems are specified to Dakota using **uncertain variables** (keywords `*_uncertain`)
- Typically generic **response functions** are used
- Thermal UQ example: here is a possible Dakota input file fragment for the uncertain variable types shown on the previous slide
- See the [Reference Manual](#) [variables section](#) for all variable types and their parameters

```
variables
  normal_uncertain 1
    descriptors      'density'
    means            8.1
    std_deviations  1.7
  lognormal_uncertain 1
    descriptors      'specific_heat'
    means            2.7
    error_factors   1.1
  poisson_uncertain
    descriptors      'fire_strength'
    lambdas          1.5
  histogram_bin_uncertain 1
    descriptors      'foam_thickness'
    num_pairs        4
    abscissas       2.5 3.0 3.5 4.0
    counts           15  11  20  0

responses
  response_functions 2
  descriptors 'pressure' 'temperature'
  ...
```

Workhorse UQ Method: Monte Carlo Sampling

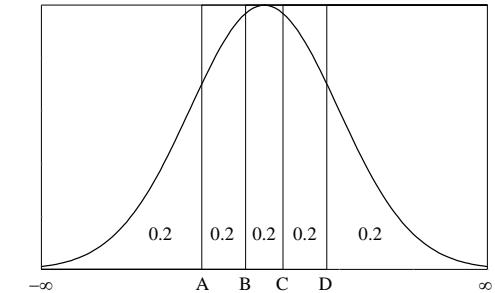
- **Sampling methods** draw (pseudo-random) realizations from the specified input distributions, run the simulation, and calculate sample statistics:
 - Sample moments, min/max, empirical PDF/CDF, based on ensemble of calculations



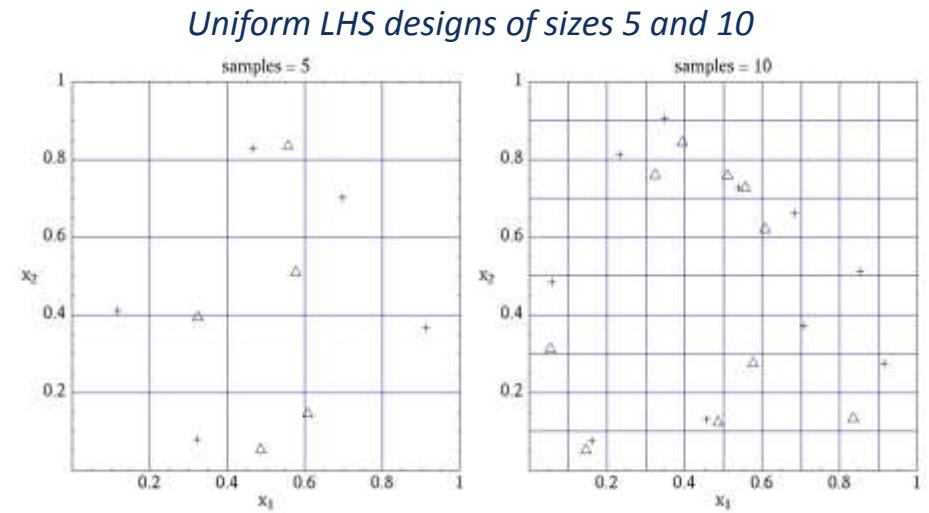
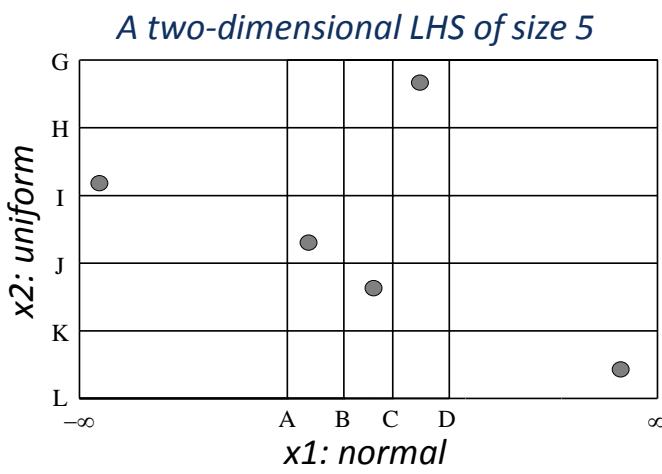
- Robust even for complex, poorly-behaved simulations
- Slow, though reliable convergence: $O(N^{-1/2})$, (in theory) independent of dimension
- Embarrassingly parallel: all samples are known at onset and can be evaluated concurrently

Latin Hypercube Sampling (LHS)

- Dakota has `sample_type` options `random` and `lhs`
- **LHS is recommended when possible**
 - Better convergence rate and stability across replicates
 - Any follow-on studies must double the sample size
- LHS (McKay and Conover): stratified random sampling among equal probability bins for all 1-D projections of an n-dimensional set of samples



example equi-probable intervals for an LHS of size 5 on a normal random variable



Exercise: LHS Sampling

Your boss announces that she can get a great deal on coat hooks from a local machine shop that happens to be owned by her brother-in-law. He unfortunately is not a very good machinist, but insists that the dimensions of most of the parts he makes are within 10% of what was requested.



Based on a design you developed earlier to support a 350 lb. horizontal load (**X**) and 500 lb. vertical load (**Y**), your boss proposes that the hooks be 5 in. long (**L**), 2 in. wide (**w**), and 2 in. thick (**t**).

Exercise: LHS Sampling

Putting aside for the moment the ethical concerns raised by your boss's obvious conflict of interest, create a sampling study in Dakota to address these questions using *Cantilever Physics*:

- Determine the variability in **stress** and **displacement** that 10% error in the dimensions (**L**, **w**, and **t**) can be expected to produce.
 - Hint 1: Produce plots of these responses vs. probability levels, i.e. cumulative distribution functions (CDFs).
 - Hint 2: Assume hook dimensions are normally distributed. Use the specified dimensions as the means and 10% of the specified dimensions as standard deviations.
- Your boss previously stipulated that the **stress** and **displacement** under load be no greater than 100,000 psi and 0.001 in., respectively. What fraction of the coat hooks produced by her brother-in-law can be expected to violate these constraints?
 - Hint: These can be read off of the CDFs, but Dakota can also estimate them for you.

Assume that Young's modulus (**E**) is 2.9e7 psi and density (**p**) is 500 lb/ft³.

Exercise materials located in ~/exercises/uncertainty_analysis/1

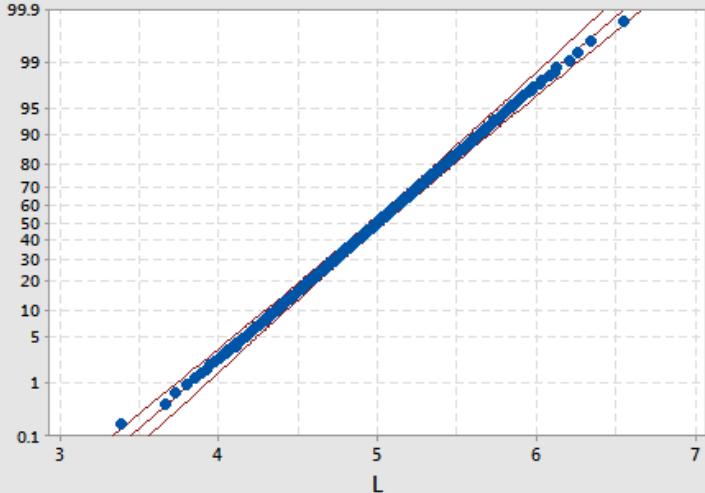
Exercise Questions

- Where do you find the relevant Dakota output?
- What statistical quantities do you find in the output?
- **Group A:** What happens if you increase/decrease the number of samples?
- **Group B:** What happens if you change the uncertainty characterization of one or more variables?

Observations

Probability Plot of L
Normal - 95% CI

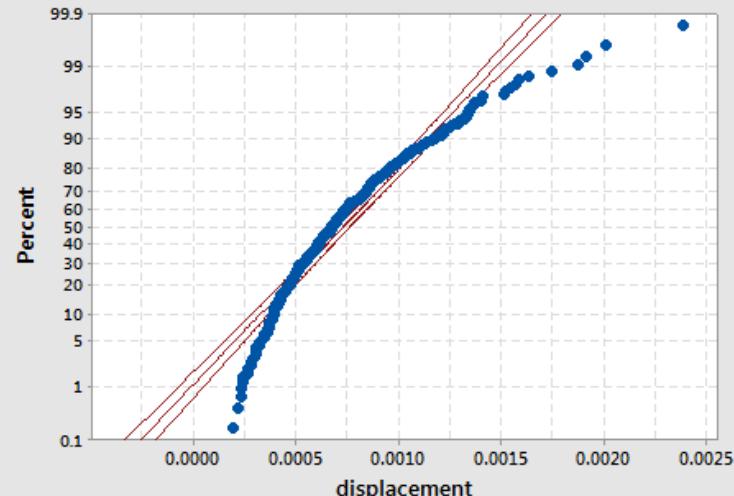
Percent



“ My variables are normally distributed. Doesn’t that mean that my responses will be, too? ”

Probability plots created in Minitab show how well the Dakota-generated sample data follow an assumed distribution (in this case normal)

Probability Plot of displacement
Normal - 95% CI



A Practical Process for UQ

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3. Characterize input uncertainties and map them into Dakota variable specifications
4. What are the model characteristics/behaviors? Recall:
 - Simulation cost, model robustness, input/output properties such as kinks, discontinuities, multi-modal, noise, disparate regimes
5. Select a method appropriate to variables, goal, and problem
6. Set up Dakota input file and interface to simulation
7. Run study and interpret the results

*covered in
other modules*

Based on variables, analysis goals, and properties, select an appropriate method...

Selecting a UQ Method

Consider variable characterizations, model properties, ultimate UQ goal to choose a method

Sampling (Monte Carlo, LHS)

- Robust, understandable, and applicable to most any model
- Slow to converge
- Moments, PDF/CDF, correlations, min/max

Stochastic Expansions

- Surrogate models tailored to UQ for continuous variables
- Highly efficient for smooth model responses
- Moments, PDF/CDF, Sobol indices

Reliability

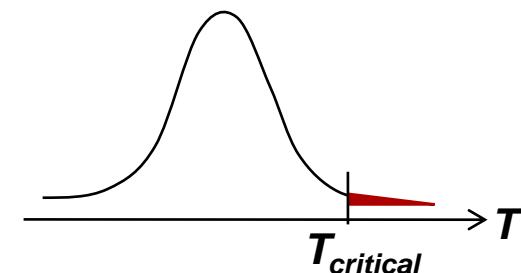
- Goal-oriented; target particular response or probability levels
- Efficient local (require derivatives) / global variants
- Moments, PDF/CDF, importance factors

Epistemic

- Non-probabilistic methods
- Generally applicable, can be costly when no surrogate
- Belief/plausibility, intervals, probability of frequency

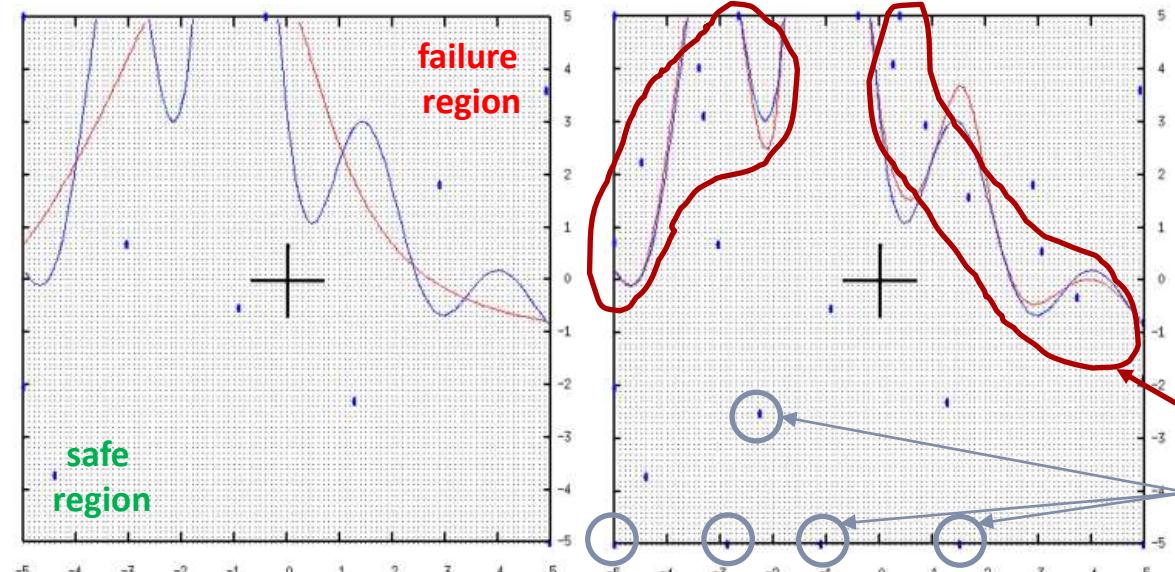
Reliability Methods: What Are They?

- Goal-oriented methods that focus on regions of probability or response space of interest, for example:
 - What temperature is achieved with 99% probability?
 - What is the probability of exceeding $T_{critical}$?
- Naïve sampling can be ineffective / under-resolved
 - Run 10,000 samples, only 5 are in relevant region
- Need to specify to Dakota
 - Probability or response threshold(s) of interest using `probability_levels`, `response_levels`
 - Method choice
 - Mean-value: best for linear problems, normally distributed parameters, efficient derivatives; specify `local_reliability` (with no `mpp_search`)
 - MPP: computes most probable point of failure when failure boundary is near linear or quadratic; specify `local_reliability` (with an `mpp_search` option)
 - Adaptive: computes probability of failure for complicated failure boundaries; specify `global_reliability`



Reliability Methods: How Do They Work?

- Reliability methods try to directly calculate statistics of interest:
 - Make simplifying approximations and/or
 - Recast the UQ as an iterative procedure, such as iteratively refined sampling or as a nonlinearly constrained optimization problem



Mean-value: uses derivatives; make a linearity (and possibly normality) assumption and project

$$\mu_T = T(\mu_u)$$

$$\sigma_T = \sum_i \sum_j Cov_u(i, j) \frac{dg}{du_i}(\mu_u) \frac{dg}{du_j}(\mu_u)$$

MPP: solve an optimization problem to directly determine input values giving rise to most probable point of failure

$$\text{minimize } u^T u$$

$$\text{subject to } T(u) = T_{critical}$$

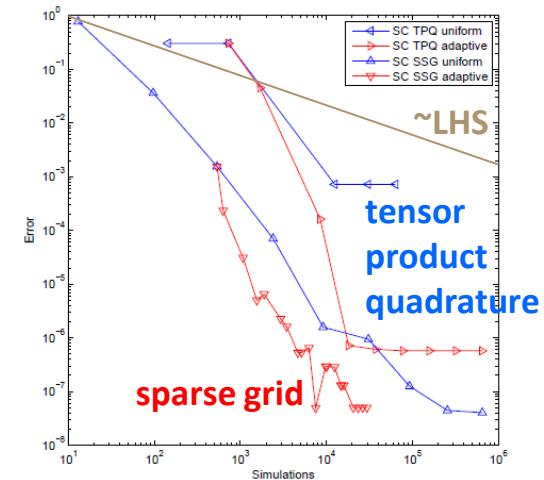
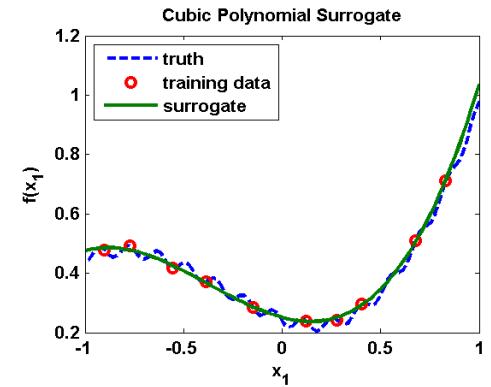
Adaptive: iteratively refine understanding of failure region

exploit

explore

Stochastic Expansions: What Are They?

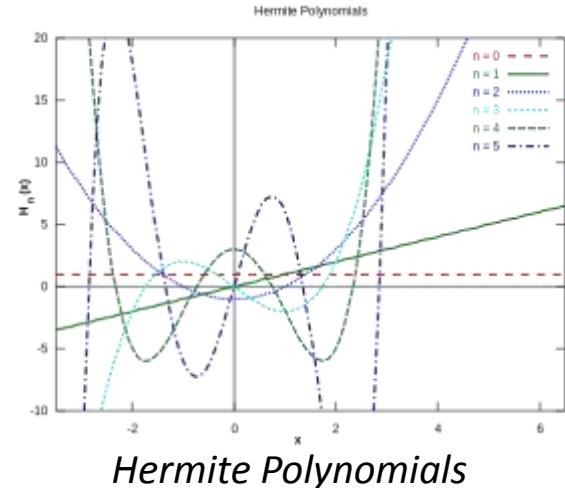
- General-purpose UQ methods that build UQ-tailored polynomial approximations of the output responses
- Perform particularly well for smooth model responses
- Resulting convergence of statistics can be considerably faster than sampling methods
- Need to specify the Dakota method:
 - Polynomial Chaos (`polynomial_chaos`): specify the type of orthogonal polynomials and coefficient estimation scheme, e.g., sparse grid or linear regression.
 - Stochastic Collocation (`stoch_collocation`): specify the type of polynomial basis and the points at which the response will be interpolated; supports piecewise local basis



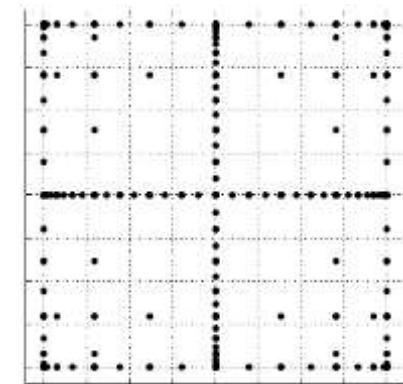
Polynomial Chaos:

How Does It Work?

- Uses an orthogonal polynomial basis $\varphi_i(u)$, e.g., Wiener-Askey basis, with Hermite polynomials orthogonal w.r.t. normal density, Legendre polynomials orthogonal w.r.t. uniform density
- Evaluates the model in a **strategic way** (sampling, quadrature, sparse grids, cubature)...
- ...to efficiently approximate the coefficients of an **orthogonal polynomial approximation** of the response
$$f(u) \approx p(u) = \sum_i c_i \varphi_i(u)$$
- And **analytically calculates statistics** from the approximation instead of approximating the statistics with MC samples



Hermite Polynomials



Sparse Grid

Selecting a UQ Method

A reasoning process: To select a Dakota method, ask yourself

- What kinds of statistics do you require on the responses
- What kinds of variables do you have and how are they characterized.
- What are the problem characteristics, including cost, robustness?
- *Get help from the Dakota team if you can't figure it out!*

Scenario 1

- Calculate probability of specific response level
- Smooth, unimodal response
- Continuous variables
- Reliable gradients

Local Reliability

Scenario 2

- Calculate mean, standard deviation
- Smooth, multimodal response
- Continuous variables
- Value-only data from previous study

Regression PCE

Dakota UQ Methods Summary

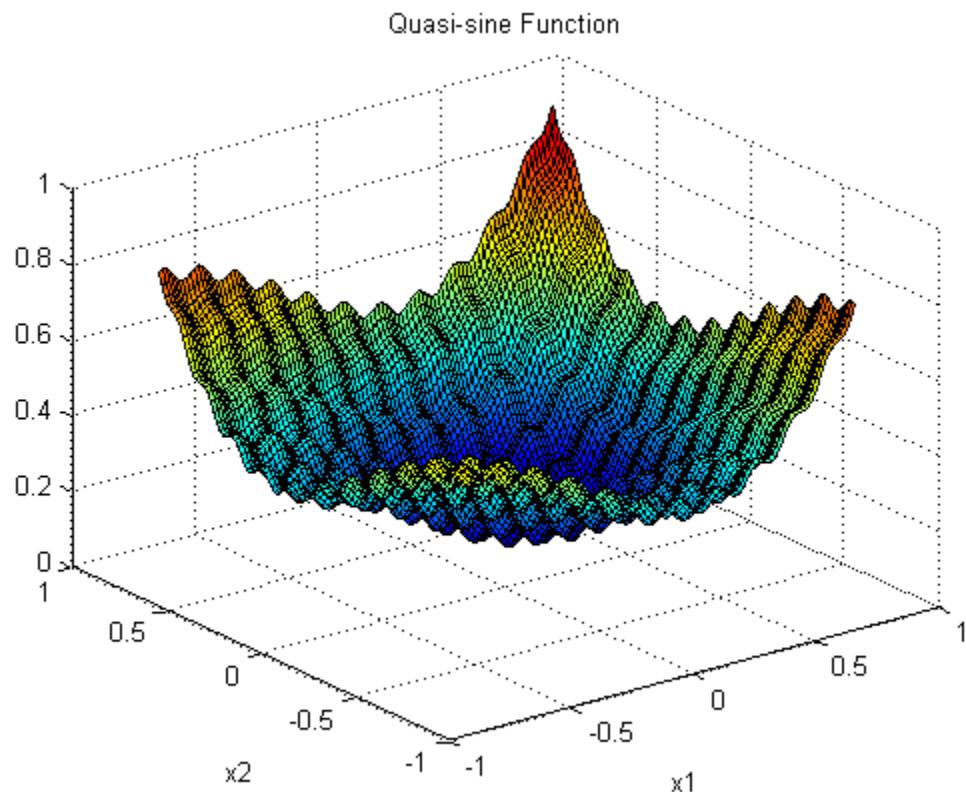


character	method class	problem character	variants
aleatory	probabilistic sampling	nonsmooth, multimodal, modest cost, # variables	Monte Carlo, LHS, importance
	local reliability	smooth, unimodal, more variables, failure modes	mean value and MPP, FORM/SORM,
	global reliability	nonsmooth, multimodal, low dimensional	EGRA
	stochastic expansions	nonsmooth, multimodal, low dimension	polynomial chaos, stochastic collocation
epistemic	interval estimation	simple intervals	global/local optim, sampling
	evidence theory	belief structures	global/local evidence
both	nested UQ	mixed aleatory / epistemic	nested

Also see Usage Guidelines in User's Manual

Exercise: Choose a method

The quasi-sine function is a multimodal function of two variables, x_1 and x_2 .



Exercise: Choose a method

Using some of the methods presented in this module, estimate the probability that the quasi-sine function is (1) less than **0.11** and (2) less than **0.30** for two cases:

- x1** and **x2** are uniformly distributed with lower bounds [-0.8, -0.8] and upper bounds [0.8, 0.8].
- x1** and **x2** obey a triangular distribution with lower bounds [-0.8, -0.8], upper bounds [0.8, 0.8], and modes [0.0, 0.0].

Before diving in, take a moment to consider which methods you expect to perform well. (Feel free to experiment with methods that you expect to perform poorly!)

Be prepared to discuss your findings. Potential observations:

- Did the distributions of the variables affect your results?
- How many function evaluations were required by the methods you chose?
- Did increasing the number of evaluations (or approximation quality, basis size, etc.) change the results?
- Did changing the initial points (for `local_reliability`) have any effect?

A partial input file is located in **~/exercises/uncertainty_analysis/2**

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What else can be done with the results?

Using Dakota-generated Data

- Users commonly work with the Dakota **tabular data file** (dakota_tabular.dat by default)
- Import tabular data into Excel, Minitab, Matlab, R, SPlus, JMP, Python to
 - Generate histogram or other probability plots
 - Generate scatterplots to assess variability or see outliers / extreme behavior
 - Fit distributions to generated model outputs
 - Post-process samples to generate other statistics, e.g., probability of failure, ANOVA, variance-based decomposition, Sobol indices, safety factors
- Use Dakota results to refine characterization of variables and repeat study
- Decision making considerations
 - Consider what form your customers needs the information in to have impact
 - Consider engaging a Dakota team member in conversation with analyst and decision maker

Common Question: UQ versus SA

What distinguishes sensitivity analysis from uncertainty analysis?

- With SA you primarily gain information about variables
 - Rank importance of parameters and characterize in what way they influence responses
 - Sometimes called inverse UQ
 - Secondarily, characterize model properties
- With UQ you primarily gain information about responses
 - Statistical properties of output responses
 - Intervals indicating bounds on response
 - Likelihood (probability of failure)
- Some methods can be used for both, e.g.,
 - LHS is often used for SA (correlations) and UQ (moments, PDFs, CDFs)
 - Polynomial chaos expansions (PCE) thought of as a UQ method, but also efficiently produce Sobol indices for ranking parameter influence

Advanced Topics Teasers

Some topics we can discuss during office hours or advanced topics modules:

- Mixed Aleatory/Epistemic UQ
- Interval analysis: sampling and optimization-based
- Probabilistic design under uncertainty
- Model form / multi-fidelity UQ
- Details on surrogates for UQ
- Treating other high-level sources of computational model uncertainty (may not be able to easily parameterize for Dakota):
 - Code implementation / software quality
 - Modelling assumptions and limitations
 - Numerical errors from discretization or other approximations
 - Data and expert judgment used to build models and inform parameter values
 - Person performing the analysis

UQ References

- SAND report 2009-3055. "Conceptual and Computational Basis for the Quantification of Margins and Uncertainty" J. Helton.
- Helton, JC, JD Johnson, CJ Sallaberry, and CB Storlie. "Survey of Sampling-Based Methods for Uncertainty and Sensitivity Analysis", *Reliability Engineering and System Safety* 91 (2006) pp. 1175-1209
- Helton JC, Davis FJ. Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems. *Reliability Engineering and System Safety* 2003;81(1):23-69.
- Haldar, A. and S. Mahadevan. *Probability, Reliability, and Statistical Methods in Engineering Design* (Chapters 7-8). Wiley, 2000.
- Eldred, M.S., "Recent Advances in Non-Intrusive Polynomial Chaos and Stochastic Collocation Methods for Uncertainty Analysis and Design," paper AIAA-2009-2274 in Proceedings of the 11th AIAA Non-Deterministic Approaches Conference, Palm Springs, CA, May 4-7, 2009.
- Dakota User's Manual: Uncertainty Quantification Capabilities
- Dakota Theory Manual
- Corresponding Reference Manual sections

Module Learning Goals

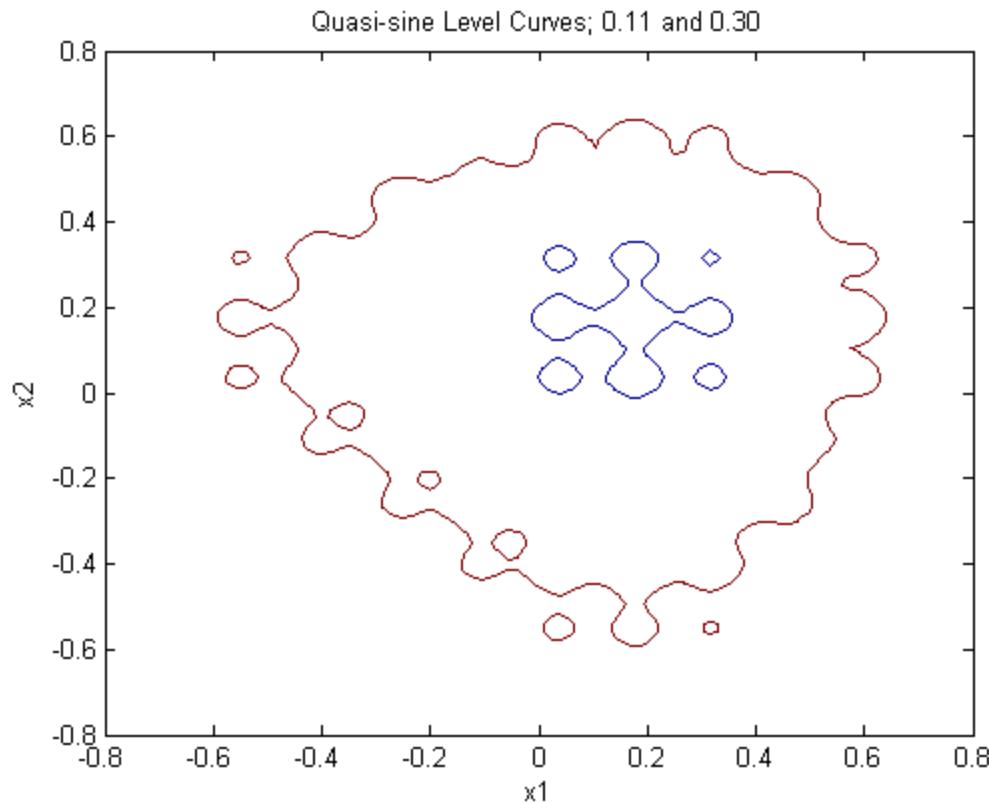
Did We Meet Them?



- Understand why you might want to perform uncertainty quantification (UQ)
- Understand prerequisites and have a practical process for UQ at your disposal
- Be able to formulate your problem, present it to Dakota, and run and understand studies
- Be able to select an appropriate Dakota UQ method
- Know how to use Dakota UQ results

BACKUP SLIDES

Quasi-sine Level Curves



Generated with Matlab

- Customers increasingly want to use simulation-based analysis for risk-informed decision making:
 - Is the simulation sufficiently representative of the real-world problem and any data?
 - How likely is my system to perform as needed? How much margin do I have?
- Ultimately, would like simulations endowed with **error bars on their output**; best estimate plus associated uncertainty
- Representative high-level sources of computational model uncertainty:
 - Code implementation / software quality
 - Modelling assumptions and limitations
 - Numerical errors from discretization or other approximations
 - Data and expert judgment used to build models and inform parameter values
 - Person performing the analysis

Method-oriented

BACKUP SLIDES

Algorithmic Strengths, Weaknesses, R&D Needs

Sampling (nongradient-based)

- *Strengths*: Simple and reliable, convergence rate is dimension-independent
- *Weaknesses*: $1/\sqrt{N}$ convergence \rightarrow expensive for accurate tail statistics

Local reliability (gradient-based)

- *Strengths*: computationally efficient, widely used, scales to large n (w/ efficient derivs.)
- *Weaknesses*: algorithmic failures for limit states with following features
 - *Nonsmooth*: fail to converge to an MPP
 - *Multimodal*: only locate one of several MPPs
 - *Highly nonlinear*: low order limit state approxs. insufficient to resolve probability at MPP

Global reliability (nongradient-based)

- *Strengths*: handles nonsmooth, multimodal, highly nonlinear limit states
- *Weaknesses*: global surrogate \rightarrow scaling to large n (*Research*: probability bias, adjoints)

Stochastic expansions (typically nongradient-based)

Strengths: functional representation, exponential convergence rates

Issues:

- Discontinuity \rightarrow Gibbs phen., slow conv.
- Singularity \rightarrow divergence in moments
- Scaling to large $n \rightarrow$ exponential growth in terms & simulation reqmts.

Research:

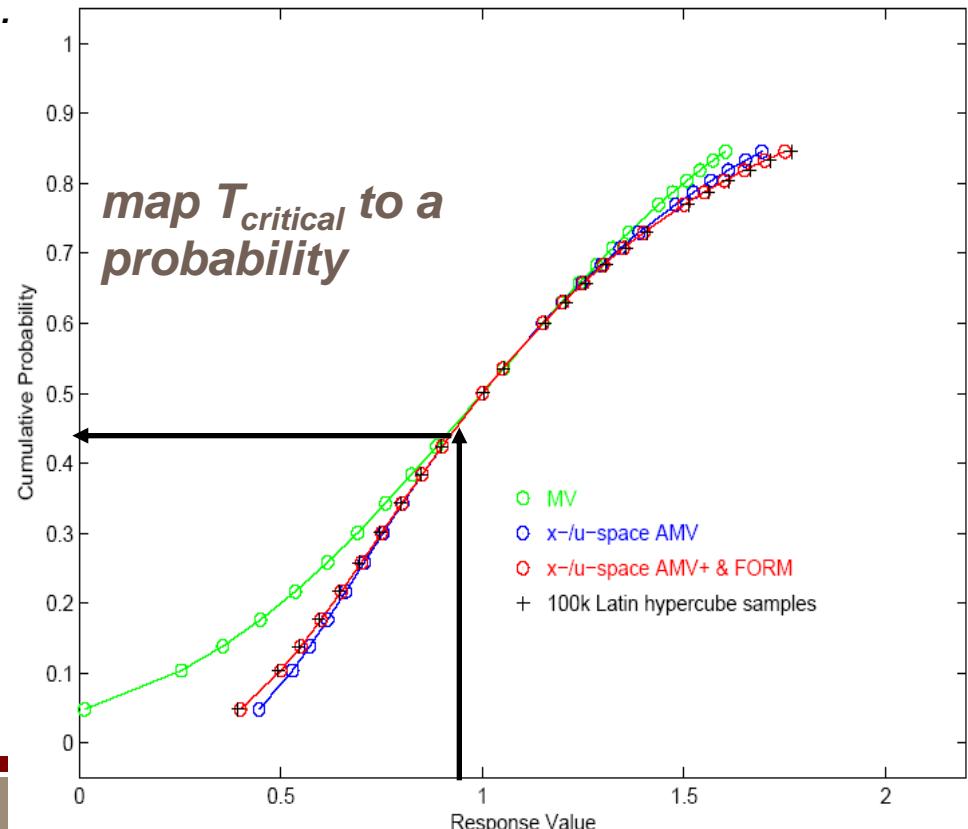
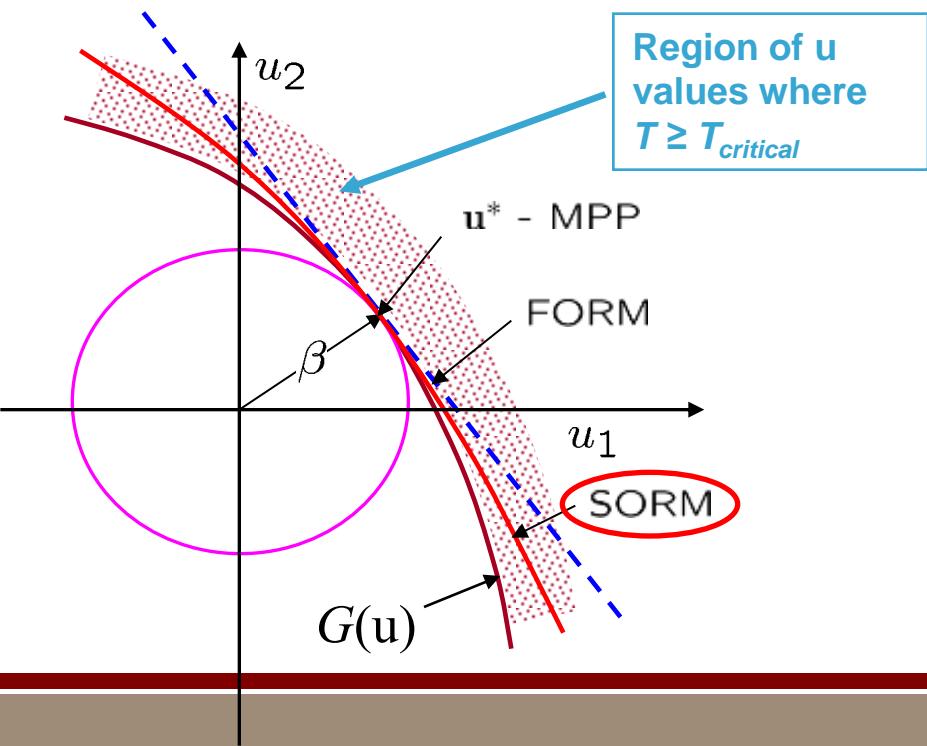
- Pade approximation
- Basis enrichment / discretization (\rightarrow local basis functions)
- p-/h-/hp-adaptive methods
- adjoint gradient-enhancement

Analytic Reliability: MPP Search

Perform optimization in uncertain variable space to determine Most Probable Point (of response or failure occurring) for $G(u) = T(u)$.

Reliability Index Approach (RIA)

minimize $\mathbf{u}^T \mathbf{u}$ *All the usual nonlinear optimization tricks apply...*
 subject to $G(\mathbf{u}) = \bar{z}$



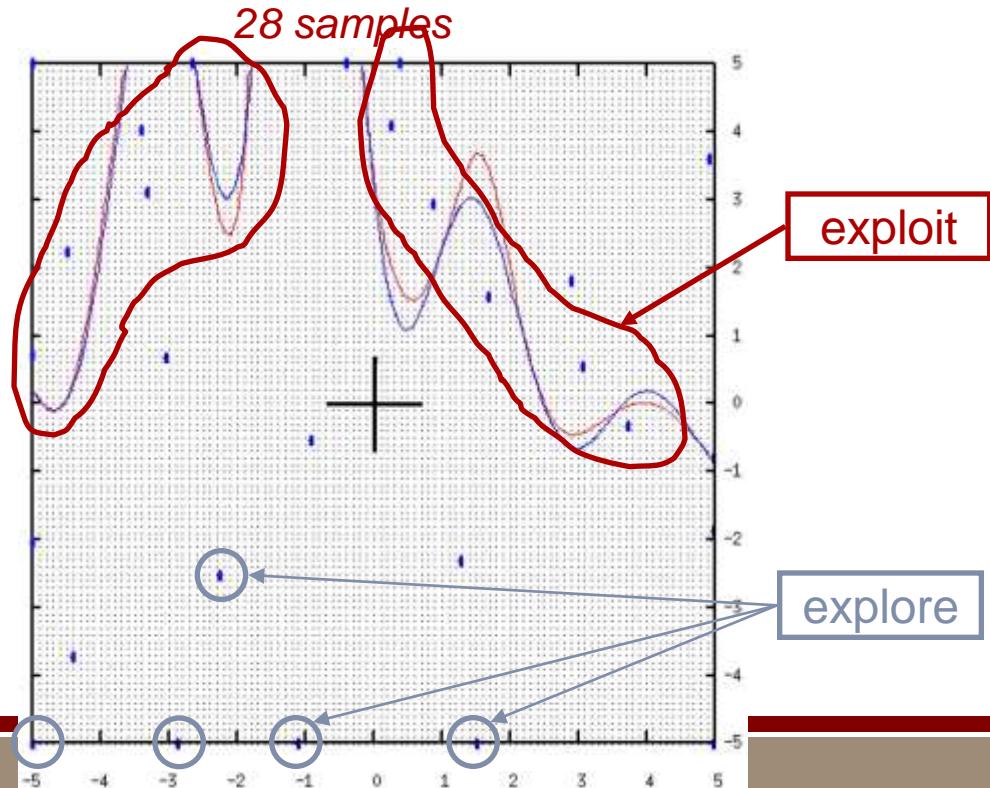
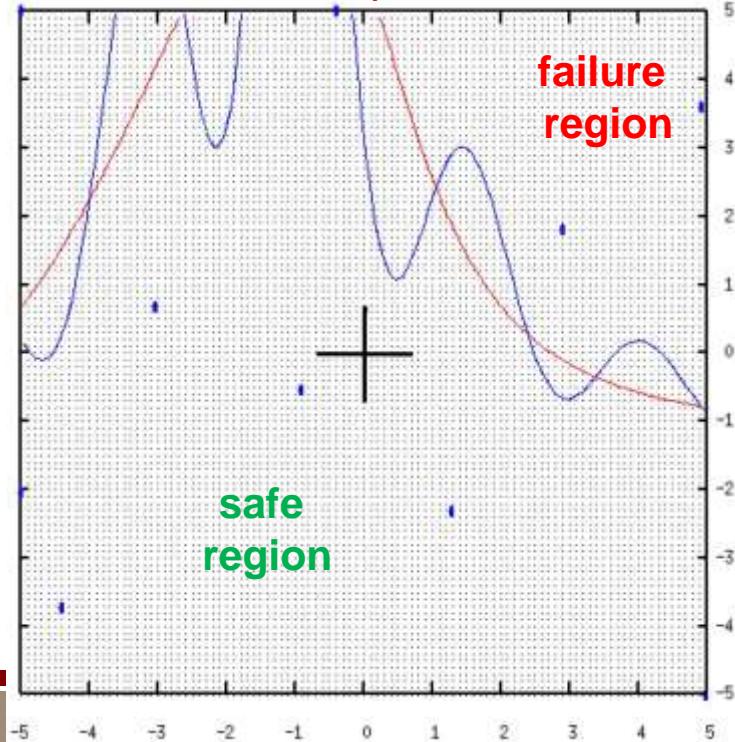
Efficient Global Reliability Analysis

Using Gaussian Process Surrogate + MMAIS



- Efficient global optimization (EGO)-like approach to solve optimization problem
- Expected feasibility function: balance exploration with local search near failure boundary to refine the GP
- Cost competitive with best local MPP search methods, yet better probability of failure estimates; addresses nonlinear and multimodal challenges

Gaussian process model (level curves) of reliability limit state with 10 samples



Generalized Polynomial Chaos Expansions (PCE)

Approximate response with Galerkin projection using multivariate orthogonal polynomial basis functions defined over standard random variables

$$R = \sum_{j=0}^P \alpha_j \Psi_j(\xi)$$

$$R(\xi) \approx f(u)$$

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R \Psi_j \varrho(\xi) d\xi$$

- Intrusive or non-intrusive
- **Wiener-Askey Generalized PCE:** optimal basis selection leads to exponential convergence of statistics

Distribution	Density function	Polynomial	Weight function	Support range
Normal	$\frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$	Hermite $He_n(x)$	$e^{-\frac{x^2}{2}}$	$[-\infty, \infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(x)$	1	$[-1, 1]$
Beta	$\frac{(1-x)^\alpha (1+x)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}$	Jacobi $P_n^{(\alpha, \beta)}(x)$	$(1-x)^\alpha (1+x)^\beta$	$[-1, 1]$
Exponential	e^{-x}	Laguerre $L_n(x)$	e^{-x}	$[0, \infty]$
Gamma	$\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}$	Generalized Laguerre $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0, \infty]$

- Can also numerically generate basis orthogonal to empirical data (PDF/histogram)

Sample Designs to Form Polynomial Chaos or Stochastic Collocation Expansions



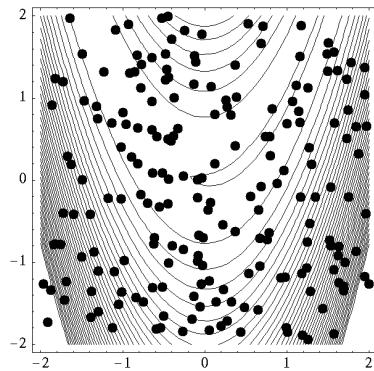
Random sampling: PCE

Expectation (sampling):

- Sample w/i distribution of x
- Compute expected value of product of R and each Y_j

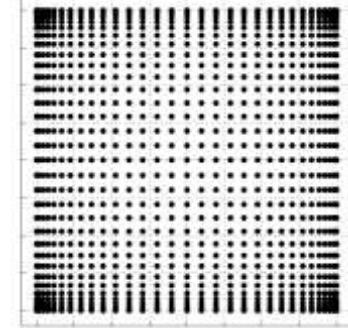
Linear regression (“point collocation”):

$$\Psi\alpha = R$$

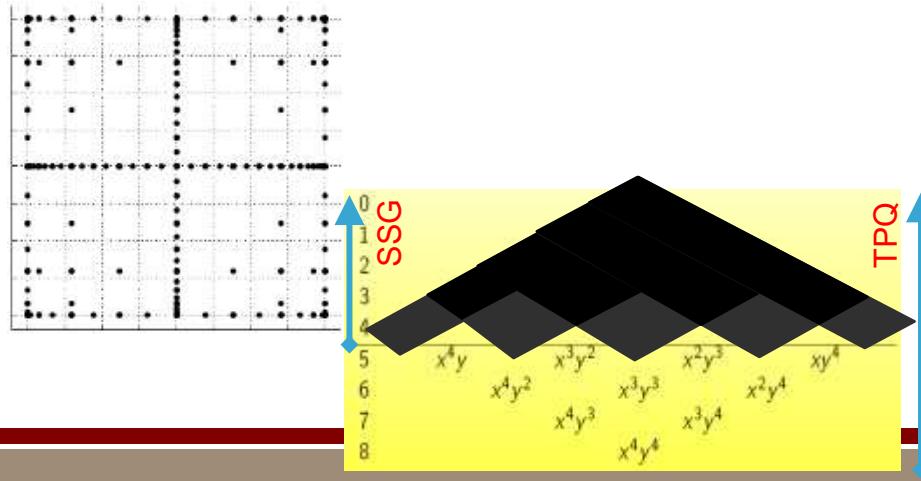


Tensor-product quadrature: PCE/SC

Tensor product of 1-D integration rules, e.g., Gaussian quadrature

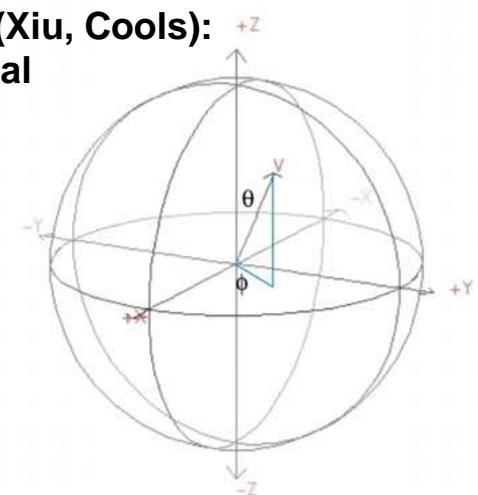


Smolyak Sparse Grid: PCE/SC



Cubature: PCE

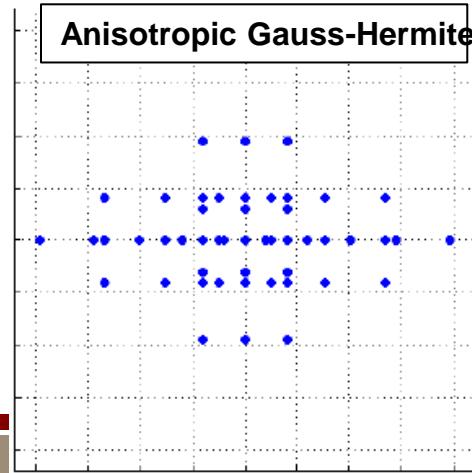
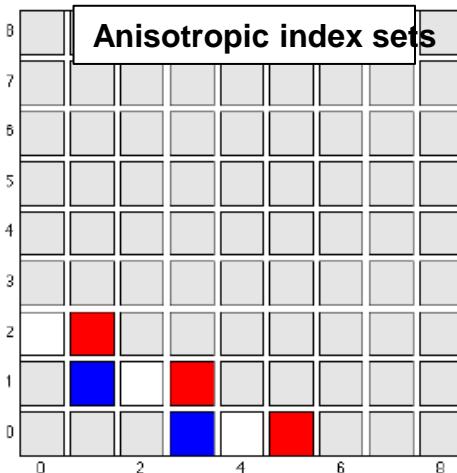
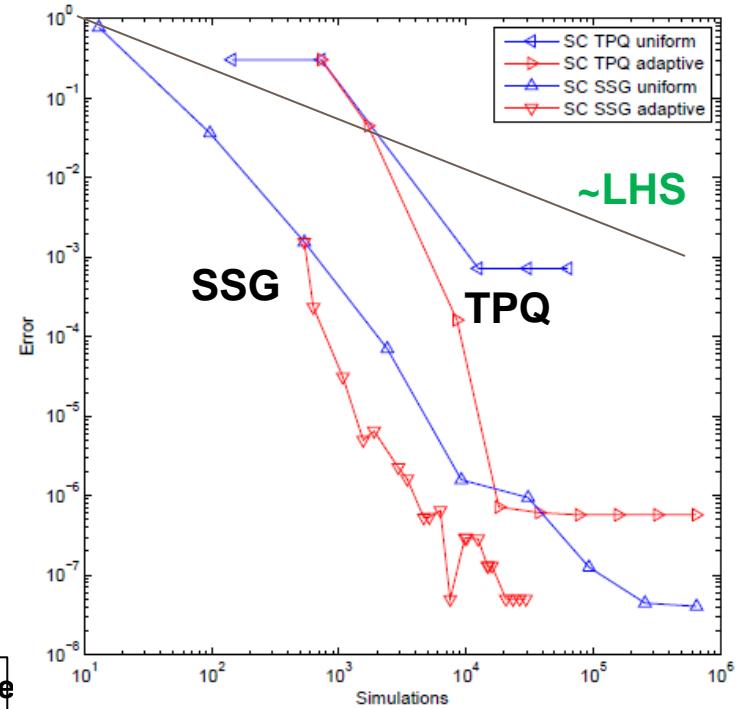
Stroud and extensions (Xiu, Cools): optimal multidimensional integration rules



Adaptive PCE/SC: Emphasize Key Dimensions

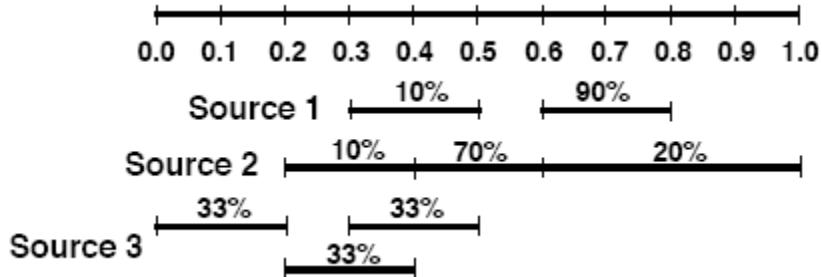


- Judicious choice of new simulation runs
- Uniform p-refinement
 - Stabilize 2-norm of covariance
- Adaptive p-refinement
 - Estimate main effects/VBD to guide
- h-adaptive: identify important regions and address discontinuities
- h/p-adaptive: p for performance; h for robustness

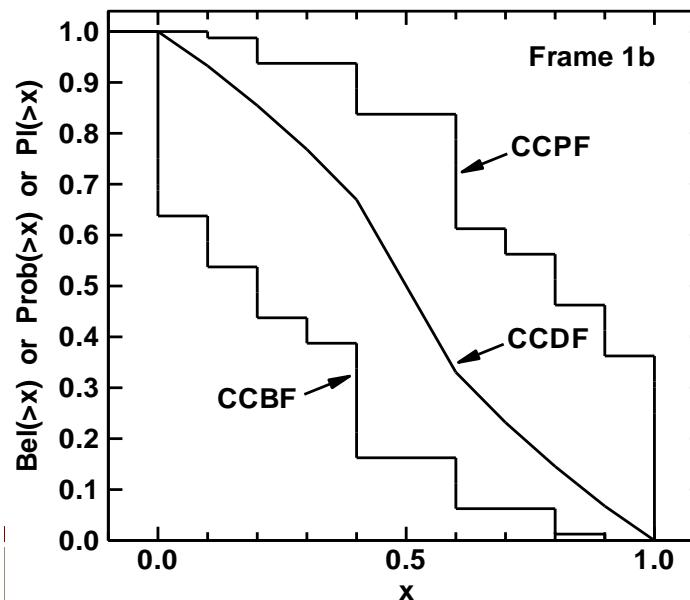
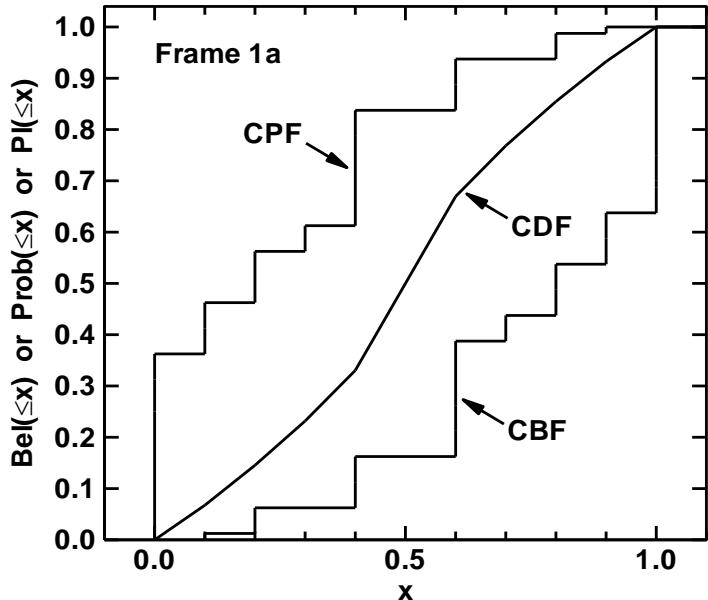


Epistemic UQ: Dempster-Shafer Theory

Intervals on the inputs are propagated to calculate

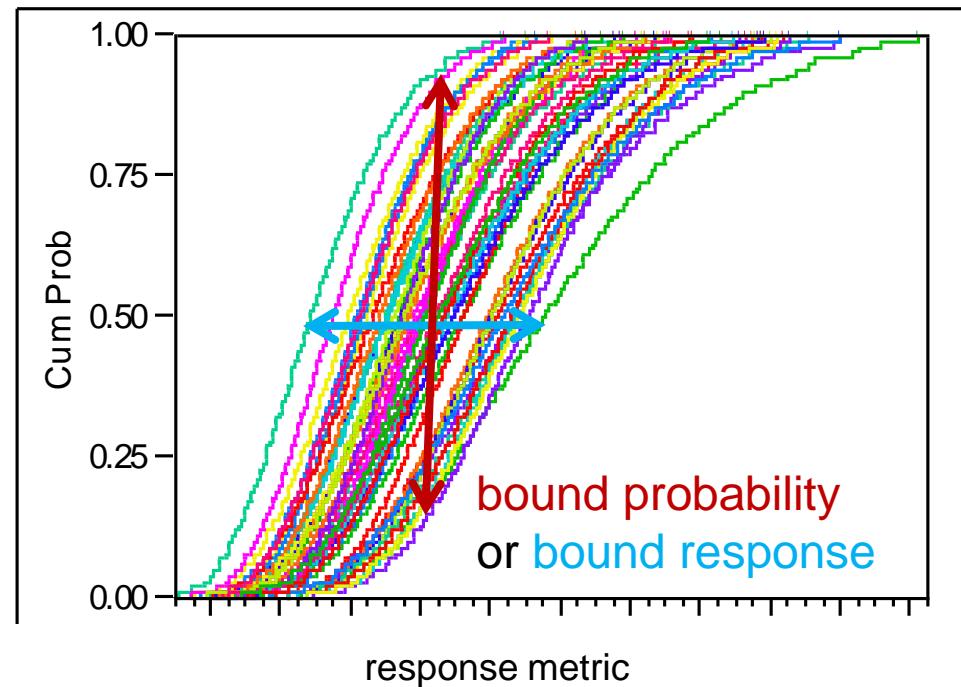
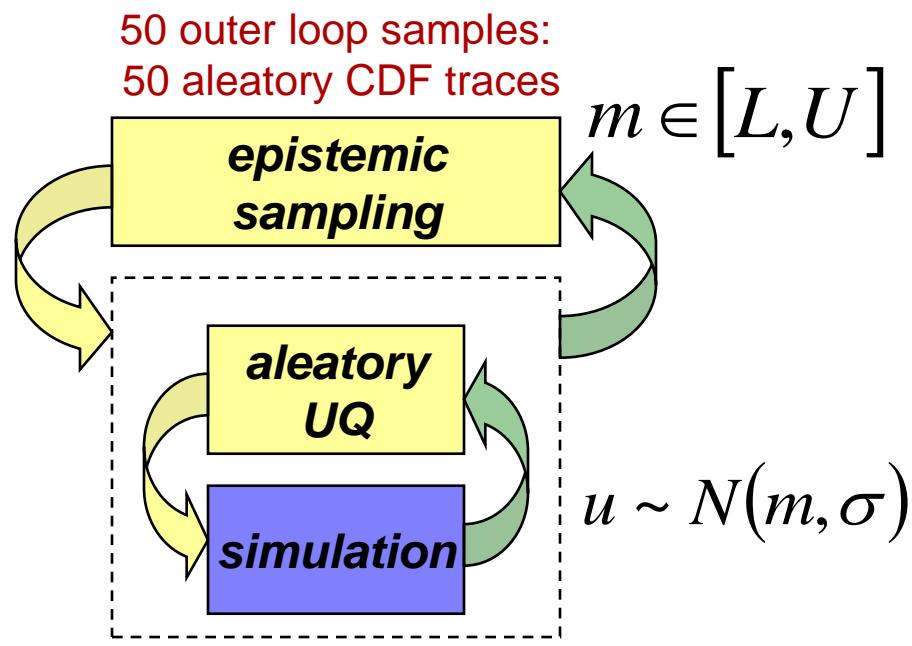


- **Belief:** a lower bound on a probability value that is consistent with the evidence
- **Plausibility:** an upper bound on a probability value that is consistent with the evidence.



Aleatory/Epistemic UQ: Nested (“Second-order”)Approaches

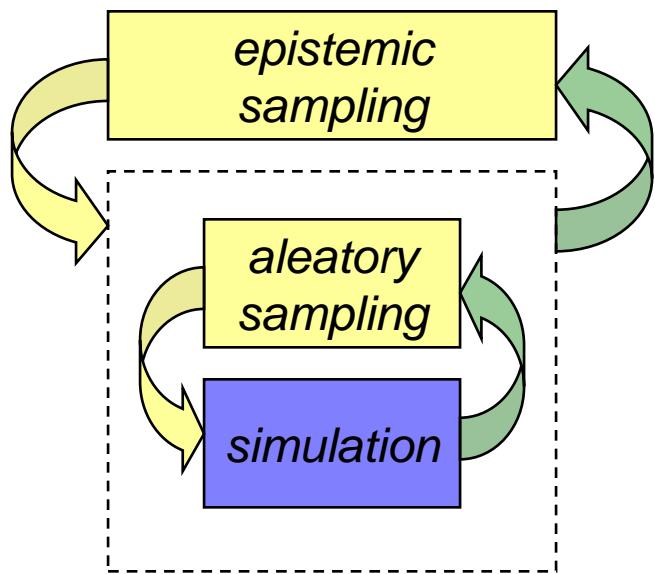
- Propagate over epistemic and aleatory uncertainty, e.g.,
UQ with bounds on the mean of a normal distribution (hyper-parameters)
- Typical in regulatory analyses (e.g., NRC, WIPP)
- Outer loop: epistemic (interval) variables, inner loop UQ over aleatory (probability) variables; *potentially costly, not conservative*
- **If treating epistemic as uniform, do not analyze probabilistically!**



“Envelope” of CDF traces represents response epistemic uncertainty

Dakota Mixed UQ with Nested Model

- Two models, each with a different set of variables
- Outer method operates on nested model
- Inner method operates on simulation model



```
method
  id_method = 'EPISTEMIC'
  model_pointer = 'EPIST_M'
  sampling sample_type lhs
  samples = 5 seed = 12347

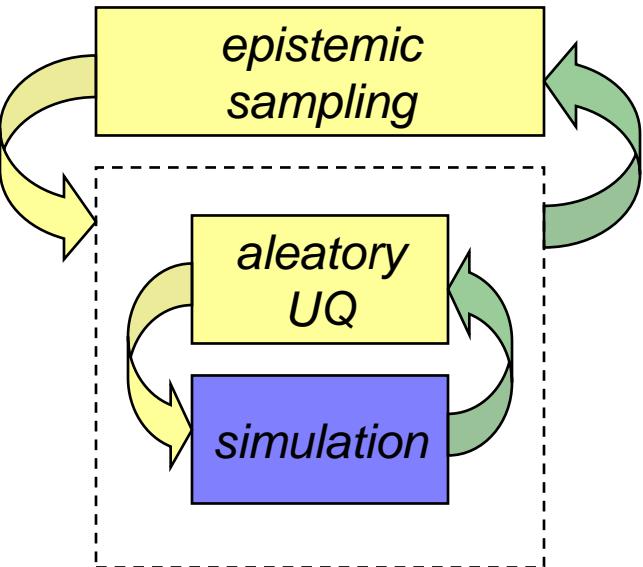
model,
  id_model = 'EPIST_M'
  nested
  variables_pointer = 'EPIST_V'
  sub_method_pointer = 'ALEATORY'
  responses_pointer = 'EPIST_R'

  primary_variable_mapping = 'X' 'Y'
  secondary_variable_mapping = 'mean' 'mean'
  primary_response_mapping = 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.
                                0. 0. 0. 0. 1. 0. 0. 0. 0. 0.
                                0. 0. 0. 0. 0. 0. 0. 0. 0. 1.

variables,
  id_variables = 'EPIST_V'
  interval_uncertain = 2
  num_intervals = 1 1
  interval_probabilities = 1.0 1.0
  upper_bounds = 600. 1200.
  lower_bounds = 400. 800.

responses,
  id_responses = 'EPIST_R'
  response_functions = 3
  descriptors ='mean_mass' '95th_perc_stress' '95th_perc_disp'
  no_gradients no_hessians
```

Example Output: Intervals on Statistics



```
<<<< Iterator nond_sampling completed.  
<<<< Function evaluation summary (ALEAT_I): 971 total (971  
new, 0 duplicate)
```

Statistics based on 50 samples:

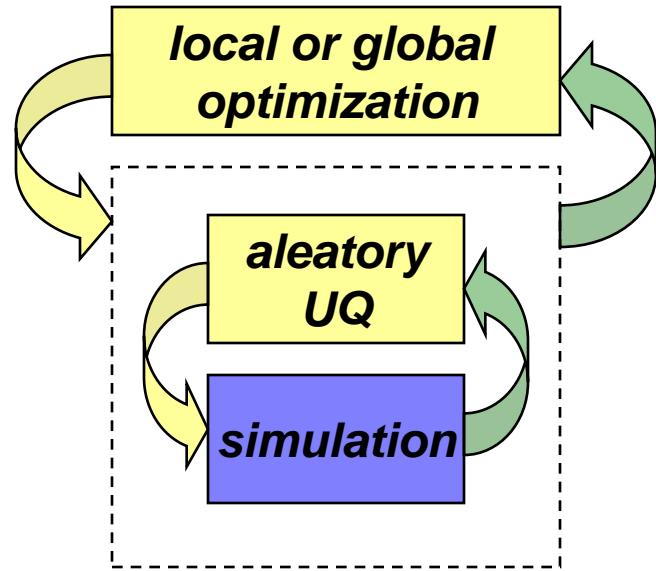
Min and Max values for each response function:

```
mean_wt: Min = 9.5209117200e+00 Max = 9.5209117200e+00  
ccdf_beta_s: Min = 1.8001336086e+00 Max = 4.0744019409e+00  
ccdf_beta_d: Min = 1.9403177486e+00 Max = 3.7628144053e+00
```

Simple Correlation Matrix between input and output:

	mean_wt	ccdf_beta_s	ccdf_beta_d
X_mean	9.40220e-16	-6.38145e-01	-9.14016e-01
Y_mean	1.38778e-15	-7.93481e-01	-4.39133e-01
...			

Interval Estimation Approach (Probability Bounds Analysis)



- *Propagate intervals through simulation code*
- **Outer loop:** determine interval on statistics, e.g., mean, variance
 - global optimization problem: find max/min of statistic of interest, given bound constrained interval variables
 - use EGO to solve 2 optimization problems with essentially one Gaussian process surrogate
- **Inner loop:** Use sampling, PCE, etc., to determine the CDFs or moments with respect to the aleatory variables

$$\min_{u_E} f_{STAT}(u_A | u_E)$$

$$u_{LB} \leq u_E \leq u_{UB}$$

$$u_A \sim F(u_A; u_E)$$

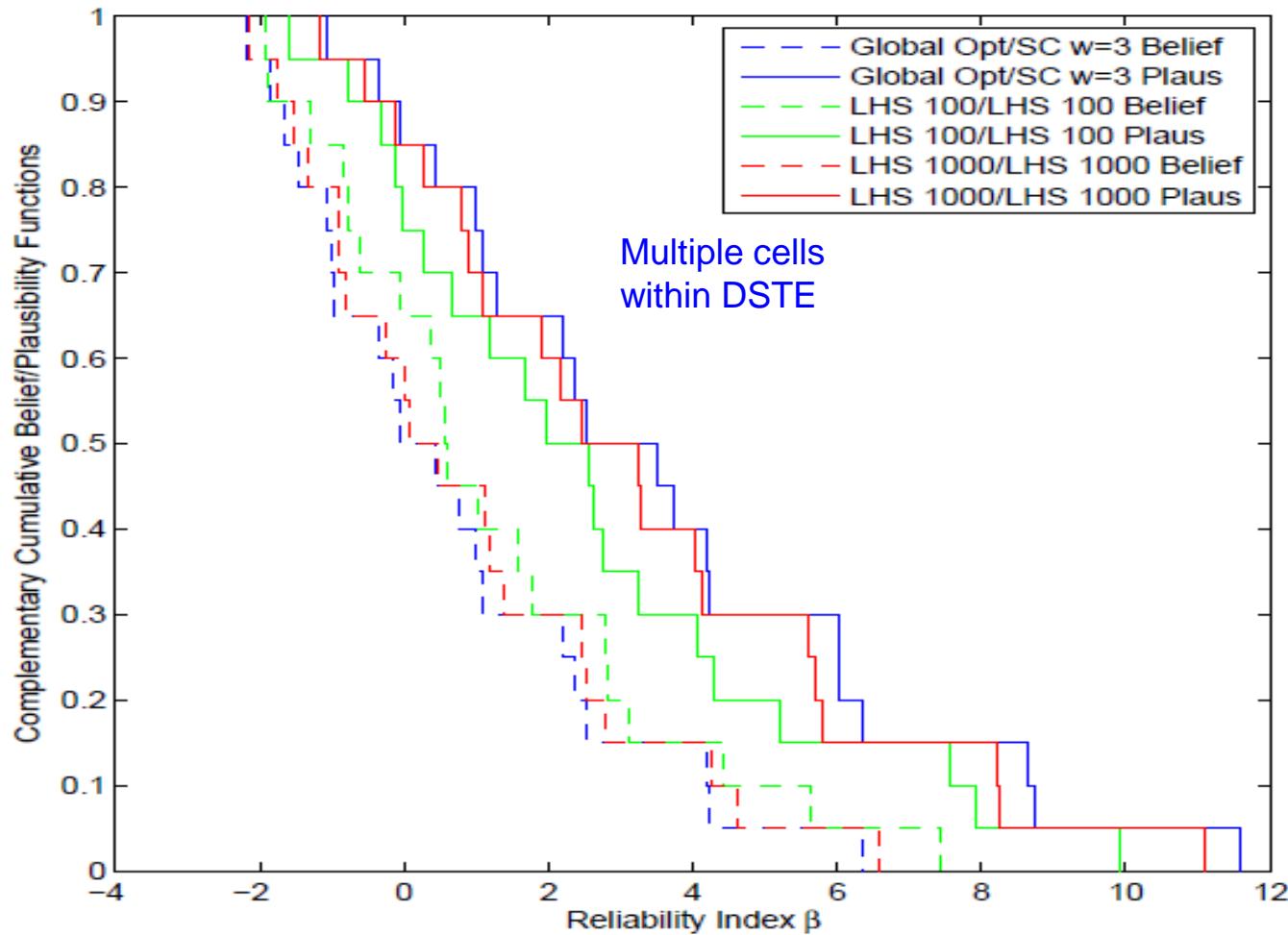
$$\max_{u_E} f_{STAT}(u_A | u_E)$$

$$u_{LB} \leq u_E \leq u_{UB}$$

$$u_A \sim F(u_A; u_E)$$

Interval Analysis can be

Tractable for Large-Scale Apps

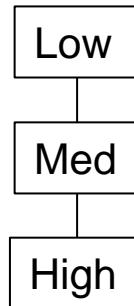


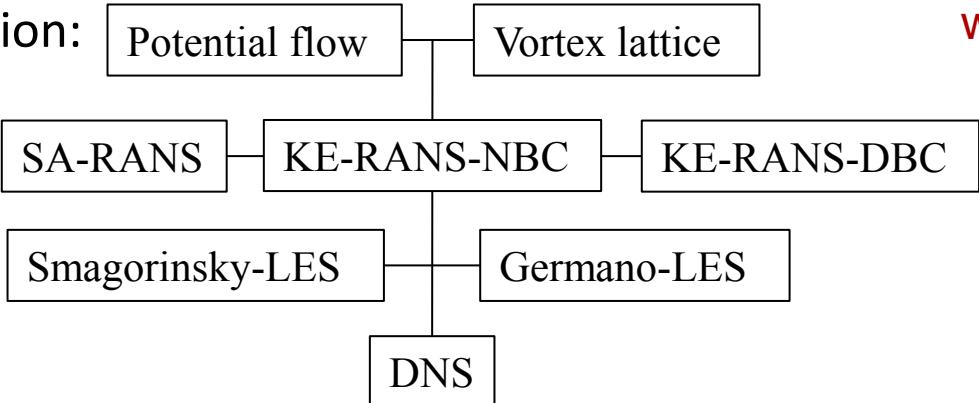
Converge to more conservative bounds with 10—100x less evaluations

Model Form UQ in Fluid/Structure Interactions

Discrete model choices for same physics:

- A clear hierarchy of fidelity (low to high)
- An ensemble of models that are all credible (lacking a clear preference structure)
 - With data: Bayesian model selection
 - Without data: epistemic model form uncertainty propagation



- Combination:
 - Potential flow
 - Vortex lattice

```
graph TD; subgraph PotentialFlow [Potential flow]; direction TB; P1[Potential flow] --- P2[Vortex lattice]; end; subgraph RANS [KE-RANS-NBC]; direction TB; R1[KE-RANS-NBC] --- R2[KE-RANS-DBC]; end; subgraph LES [Smagorinsky-LES / Germano-LES]; direction TB; L1[Smagorinsky-LES] --- L2[Germano-LES]; end; subgraph DNS [DNS]; direction TB; DNS[DNS] --- LES; end; PotentialFlow --- RANS; RANS --- LES; LES --- DNS
```

wind turbine applications

Multifidelity UQ using Stochastic Expansions

- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity “design” codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

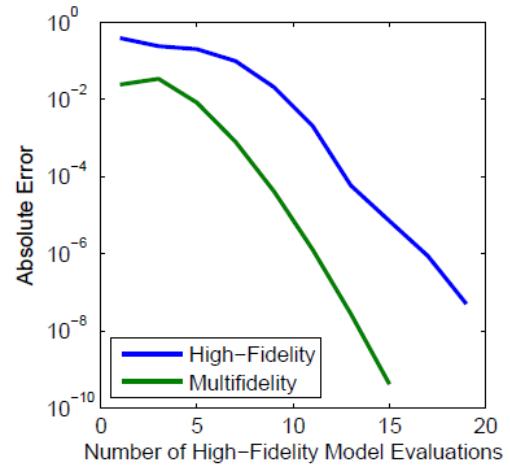
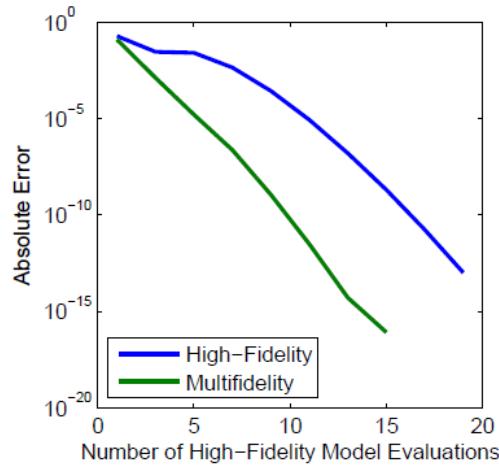
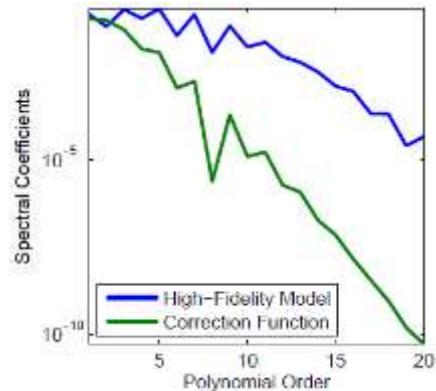
$$\hat{f}_{hi}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) \mathbf{L}_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) \mathbf{L}_j(\xi)$$

$$N_{lo} \gg N_{hi}$$

$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi - 0.5e^{-0.02(\xi-5)^2}$$

$$R_{\text{low}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi,$$

discrepancy



Low fidelity

CACTUS: Code for Axial and Crossflow Turbine Simulation

High fidelity: DG formulation for LES
Full Computational Fluid Dynamics/
Fluid-Structure Interaction

Uncertainty Quantification not Addressed Here

- Efficient epistemic UQ **[Dakota]**
- Fuzzy sets (Zadeh)
- Imprecise Probability (Walley)
- Dempster-Shafer Theory of Evidence (Klir, Oberkampf, Ferson) **[Dakota]**
- Possibility theory (Joslyn)
- Probability bounds analysis (p-boxes)
- Info-gap analysis (Ben-Haim)

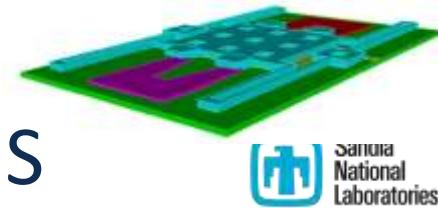
- Bayesian model calibration / inference via MCMC **[Dakota]**
- Other Bayesian approaches: Bayesian belief networks, Bayesian updating, Robust Bayes, etc.
- Scenario evaluation

(Some available in **[Dakota]**)

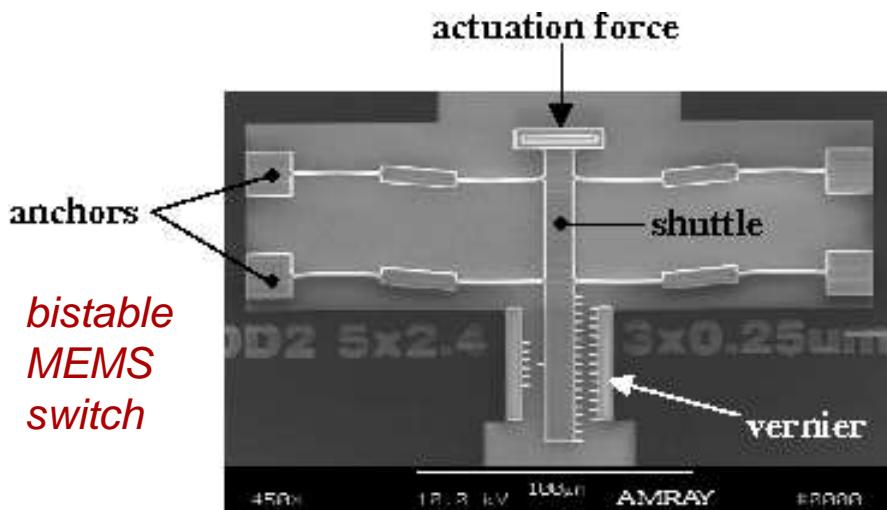
Application-oriented

BACKUP SLIDES

Nondeterministic Design: Shape Optimization of Compliant MEMS



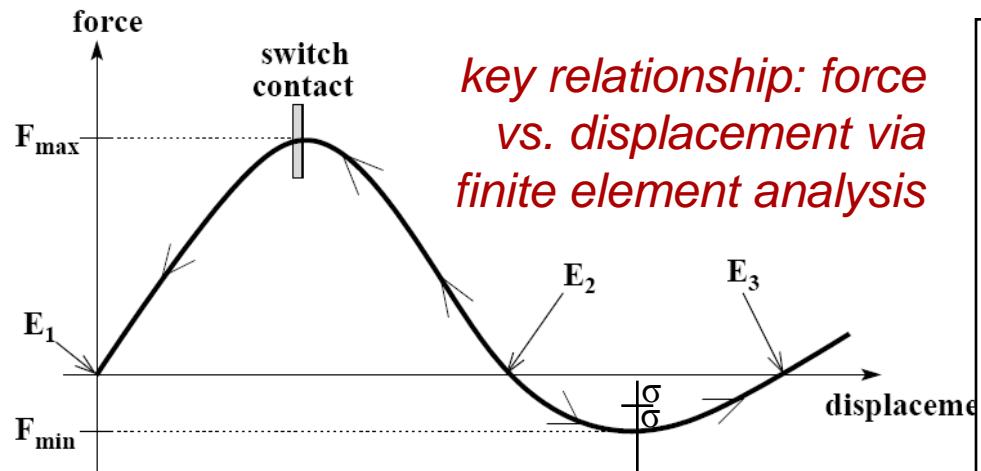
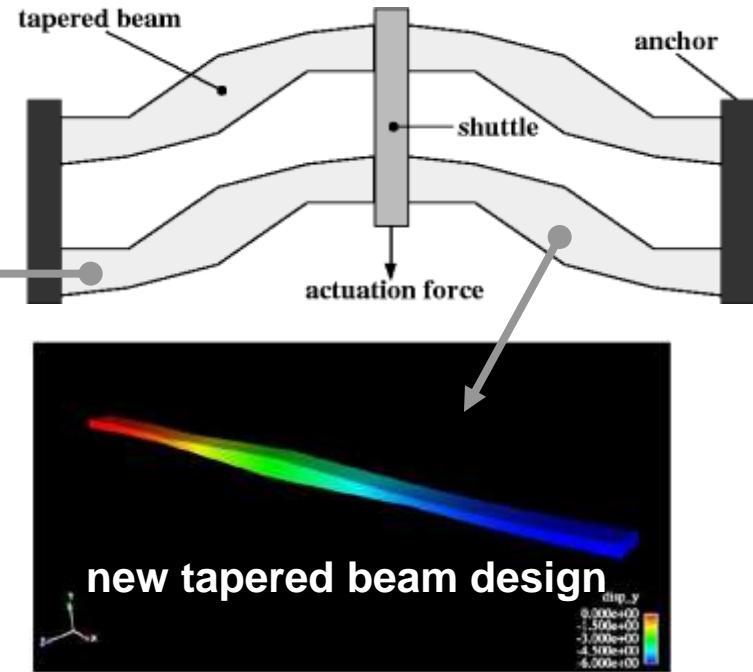
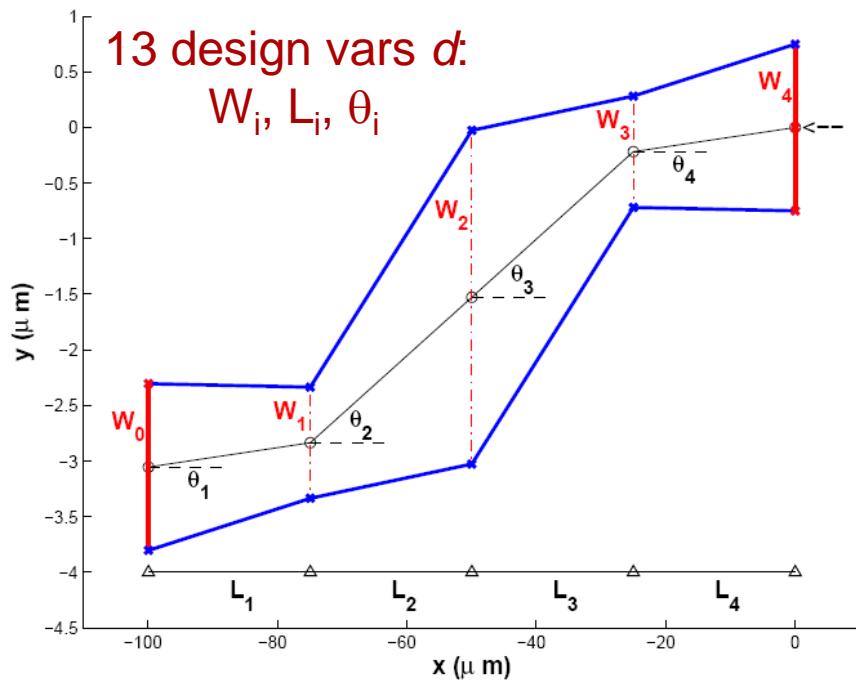
- **Micro-electromechanical system (MEMS):** typically made from silicon, polymers, or metals; used as micro-scale sensors, actuators, switches, and machines
- **MEMS designs:** subject to substantial variability, lack historical knowledge base; uncertainty from materials, micromachining, photo lithography, etching process
- Resulting part yields can be low or have poor cycle durability
- **Goal:** shape optimize finite element model of bistable switch to...
 - Achieve prescribed reliability in actuation force
 - Minimize sensitivity to uncertainties (robustness)



*uncertainties to be considered
(edge bias and residual stress)*

variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

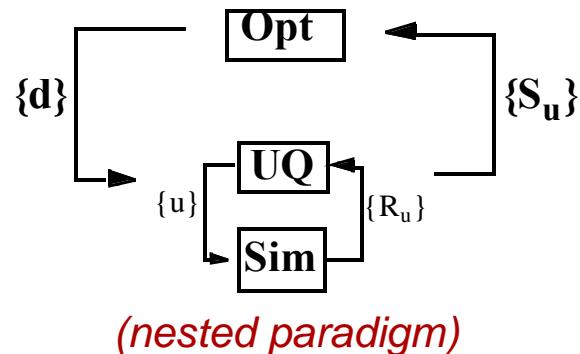
MEMS Switch Design: Geometry Optimization



- Typical design specifications:**
- actuation force F_{\min} reliably $5 \mu\text{N}$
 - bistable ($F_{\max} > 0, F_{\min} < 0$)
 - maximum force: $50 < F_{\max} < 150$
 - equilibrium $E2 < 8 \mu\text{m}$
 - maximum stress < 1200 MPa

Optimization Under Uncertainty

Rather than design and then post-process to evaluate uncertainty...
actively design optimize while accounting for uncertainty/reliability metrics $s_u(d)$,
 e.g., mean, variance, reliability, probability:

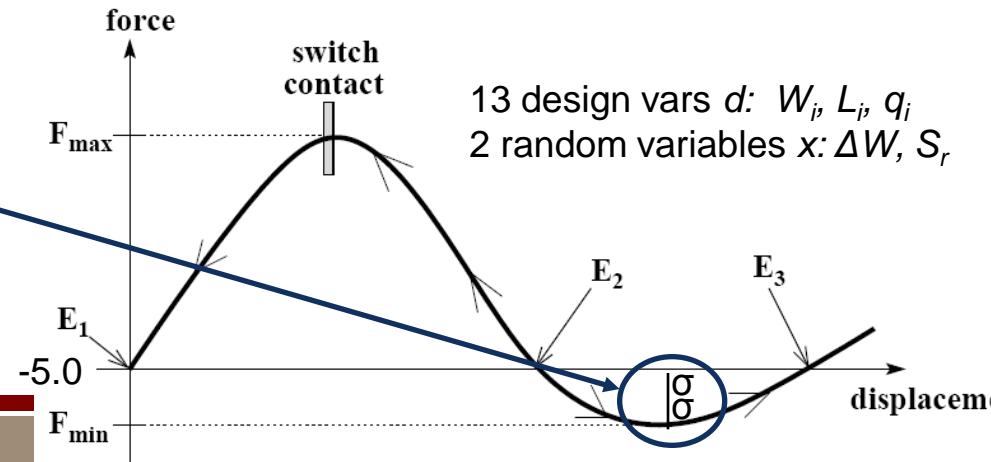


$$\begin{aligned}
 & \min f(d) + W s_u(d) \\
 \text{s.t.} \quad & g_l \leq g(d) \leq g_u \\
 & h(d) = h_t \\
 & d_l \leq d \leq d_u \\
 & a_l \leq A_i s_u(d) \leq a_u \\
 & A_e s_u(d) = a_t
 \end{aligned}$$

Bistable switch problem formulation (Reliability-Based Design Optimization):

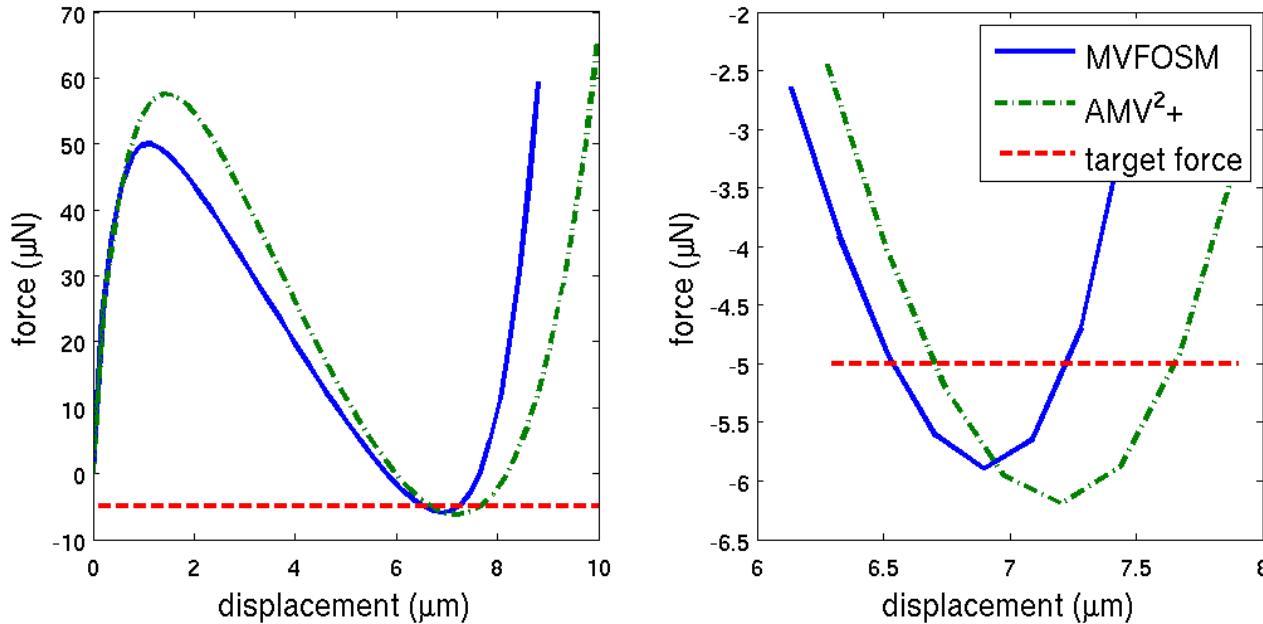
simultaneously reliable and robust designs

$$\begin{aligned}
 \max \quad & \mathbb{E}[F_{min}(d, x)] \\
 \text{s.t.} \quad & 2 \leq \beta_{ccdf}(d) \\
 & 50 \leq \mathbb{E}[F_{max}(d, x)] \leq 150 \\
 & \mathbb{E}[E_2(d, x)] \leq 8 \\
 & \mathbb{E}[S_{max}(d, x)] \leq 3000
 \end{aligned}$$



Reliability-based Design Optimization

Finds Optimal & Robust Design



Close-coupled results: DIRECT / CONMIN + reliability method yield optimal and reliable/robust design:

metric			initial \mathbf{d}^0	MVFOSM	AMV^2+	FORM
l.b.	name	u.b.		optimal \mathbf{d}_M^*	optimal \mathbf{d}_A^*	optimal \mathbf{d}_F^*
	$E[F_{min}] (\mu\text{N})$		-26.29	-5.896	-6.188	-6.292
2	β		5.376	2.000	1.998	1.999
50	$E[F_{max}] (\mu\text{N})$	150	68.69	50.01	57.67	57.33
	$E[E_2] (\mu\text{m})$	8	4.010	5.804	5.990	6.008
	$E[S_{max}] (\text{MPa})$	1200	470	1563	1333	1329
	AMV ² + verified β		3.771	1.804	-	-
	FORM verified β		3.771	1.707	1.784	-