SAND2012-7387P

DAKOTA 101

Uncertainty Quantification

http://dakota.sandia.gov

Learning Goals: Uncertainty Quantification

- Understand why you need to consider uncertainties in modeling and simulation
- Explain how UQ works, and what data and choices are required to perform it
- Be able to enumerate uncertainties in your domain and ways uncertainty-endowed code predictions could help decision making
- Create DAKOTA studies to perform UQ (sampling, reliability, stochastic expansions, epistemic)
- Understand DAKOTA statistics outputs and margin assessment
- How to choose from UQ options in DAKOTA for your problem

Why Perform Uncertainty Quantification?

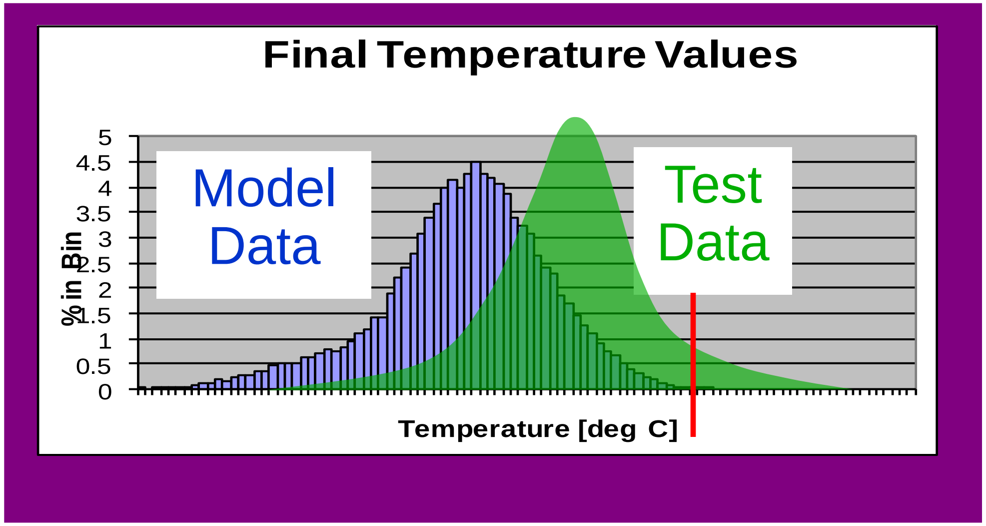
- What? Determine variability, distributions, statistics of code outputs, given uncertainty in input factors
- Why? Assess likelihood of typical or extreme outcomes. Given input uncertainty…
  - Determine mean or median performance of a system
  - Assess variability in model response
  - Find probability of reaching failure/success criteria (reliability metrics)
  - Assess range/intervals of possible outcomes
- 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)

Uncertainties in Simulation and Validation

Parameterized…

A *few* uncertainties affecting computational model output/results:

- physics/science parameters
- statistical variation, inherent randomness
- model form / accuracy
- material properties
- manufacturing quality
- operating environment, interference
- initial, boundary conditions; forcing
- geometry / structure / connectivity
- experimental error (measurement error, measurement bias)
- numerical accuracy (mesh, solvers); approximation error
- human reliability, subjective judgment, linguistic imprecision

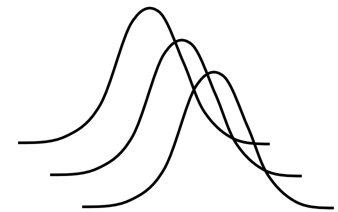


The effect of these on model outputs should be integral to an analyst's deliverable: *best estimate PLUS uncertainty!*

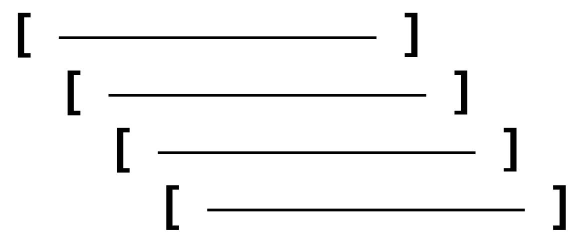
Categories of Uncertainty

Needed for characterizing uncertainty and selecting algorithms

- **Aleatory *(think probability density function; 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 or unknown distro parm)***
  - **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**



- ***See Rich Hills' course on aleatory vs. epistemic uncertainty***

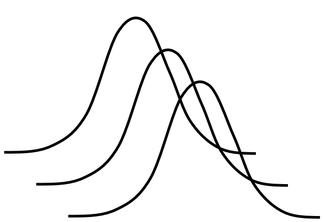
Mechanics of (Parametric) Uncertainty Quantification

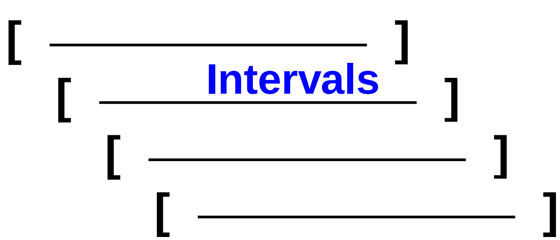
- **Identify and characterize uncertain variables (may not be normal, uniform)**
- ***Forward propagate: quantify the effect that (potentially correlated) uncertain (nondeterministic) input variables have on model output:***

Input Variables *u* **(physics parameters, geometry, initial and boundary conditions)** → **Computational Model** → **Variable Performance Measures *f(u)***

Uncertainties on inputs

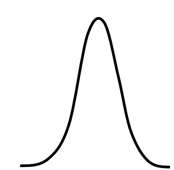
- **Parameterized distributions: normal, uniform, gumbel, etc.**
- **Means, standard deviations**
- **PDF, CDF from data**
- **Intervals**
- **Belief structures**





Uncertainties on outputs

- **Means, standard deviations**
- **Probabilities**
- **Reliabilities**
- **PDF, CDF**
- **Intervals**
- **Belief, plausibility**

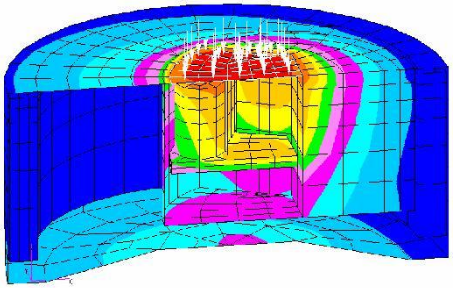


Why the Recent UQ Buzz?

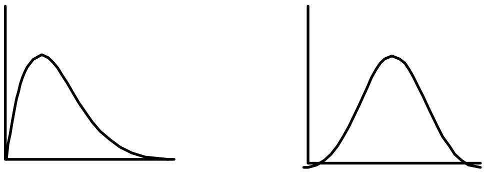
DOE in general, ASC V&V perspective in particular, however evident across sectors

- **Shift from test-based to M&S-based design and certification**
- **Supporting risk-informed decision-making requires credible M&S:**
  - ***Predictive simulations:* verified, validated for application domain of interest**
  - ***Quantified uncertainties:* random variability effect is understood**
- **DOE Quantification of Margins and Uncertainties (QMU) demands *best estimate* + *uncertainty* in the decision-making context**
- **UQ is a especially critical when we cannot test, e.g., nuclear weapon stockpile stewardship, climate science, genetics**

Example: Thermal Uncertainty Quantification

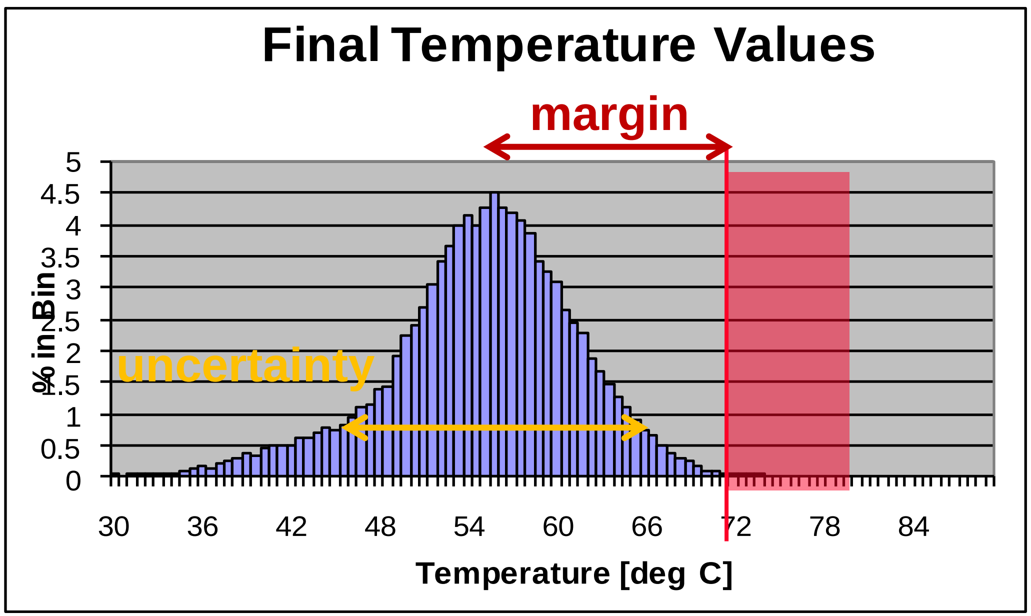


- **Device subject to heating** (experiment or computational simulation)
- **Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by** $u_1, \ldots, u_N$
- **Response temperature** $f(u)=T(u_1, \ldots, u_N)$ **calculated by heat transfer code**



Given distributions of $u_1,\ldots,u_N$*, UQ methods calculate statistical info on outputs:*

- **Mean(*T*), StdDev(*T*), Probability(**$T \geq T_{critical}$**)**
- **Probability distribution of temperatures**
- ***Correlations (trends) and sensitivity of temperature***



Group Discussion: Uncertainty in Your Domain

- What sources of uncertainty should you consider in your analysis-based decision making?
- How do you account for their effect today?
- Which of these directly affect the simulations in your analysis process?
- Do you consider the uncertainties aleatory or epistemic?
- What data are available to characterize the uncertain factors?

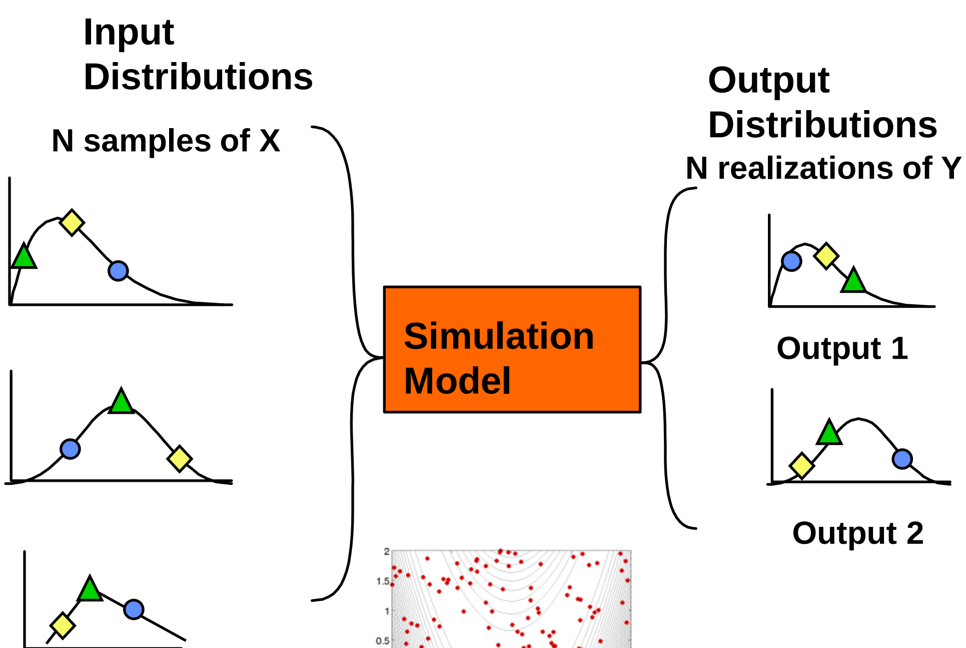
Three Contrasting DAKOTA UQ Methods

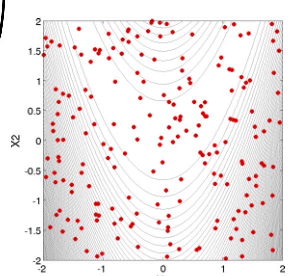
- **Sampling (Monte Carlo, Latin hypercube):** **robust, easy to understand, slow to converge / resolve statistics**
- **Reliability: good at calculating probability of a particular behavior or failure / tail statistics; efficient, some methods are only local**
- **Stochastic Expansions (PCE/SC global approximations): efficient tailored surrogates, statistics often derived analytically, far more efficient than sampling for reasonably smooth functions**

- ***Recent DAKOTA research largely focuses on advanced UQ methods transcending traditional Monte Carlo methods, including reliability, stochastic expansions, and evidence/interval to make these practical for a range of model costs and characterizations of uncertainty***

Prevalent UQ Method: Random Sampling

- Assume distributions on each of the *n* uncertain input variables
- Sample from each distribution and pair into *N* samples
- Run the simulation model for each of the *N* samples
- Use results ensemble to build up a distribution for each of the *m* outputs





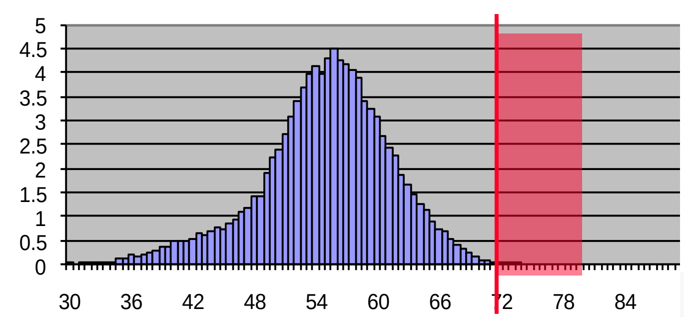
- sample mean

$$\bar{T} = \frac{1}{N} \sum_{i=1}^{N} T(u^i)$$

- sample variance

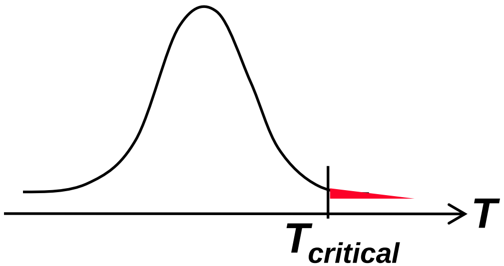
$$T_{\sigma^2} = \frac{1}{N} \sum_{i=1}^{N} \left[T(u^i) - \bar{T} \right]^2$$

- full PDF(probabilities)



Calculating (Potentially Small) Probability of Failure

- **Given uncertainty in materials, geometry, and environment, how to determine likelihood of failure: *Probability($T \geq T_{critical}$)?***
- **Perform 10,000 LHS samples and count how many exceed threshold;**
  (better) perform adaptive importance sampling



Mean value: **make a linearity (and possibly normality) assumption and project;**
great for many parameters with efficient derivatives!

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

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

Reliability: **directly determine input variables which give rise to failure behaviors by solving an optimization problem for a most probable point (MPP) of failure**

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

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

All the usual nonlinear optimization tricks apply…

Generalized Polynomial Chaos Expansions (PCE)

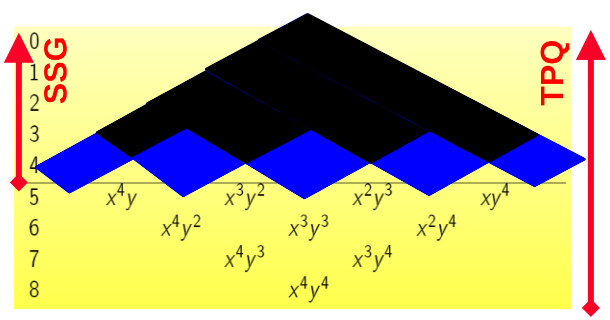
Approximate response with Galerkin projection using global multivariate orthogonal polynomial basis functions defined over standard random variables

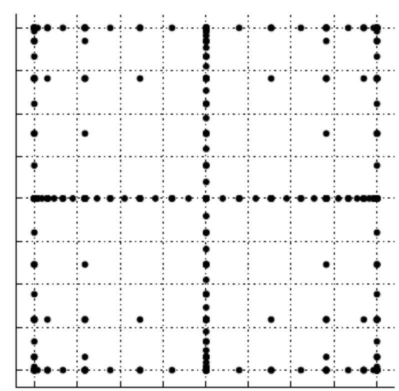
$$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi)$$

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

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

- **One approximated, calculate statistics (and sensitivities) analytical, or sample the cheaper surrogate.**
- **Wiener-Askey Generalized PCE: optimal polynomial basis leads to exponential convergence of statistics (Normal/Hermite, Uniform/Legendre)**
- **For empirical data: numerically generate basis orthogonal to histogram**
- **Many variants for integration, adaptivity**





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Group Discussion / Exercise

- **Locate in the reference manual:**
  - **method options for sampling, reliability, and polynomial chaos**
  - **uncertain variable specifications**
- **Assume the following uncertain variable characterizations for the cantilever beam**
  - **Yield stress** R **~ Normal(40000, 2000)**
  - **Young's modulus** E **~ Normal(2.9e7, 1.45e6)**
  - **Horizontal load** X **~ Normal(500, 100)**
  - **Vertical load** Y **~ Normal(1000, 100)**
  - **width** w **and thickness** t **both fixed at 2.5**
- **What are some uncertainty quantification questions you might ask about the outputs of cantilever analysis?**
- **Use JAGUAR (or discuss how) to create a DAKOTA input to perform a UQ sampling study for cantilever.**

Class Exercise: Cantilever Beam UQ with Sampling

- Perform UQ with LHS method on `mod_cantilever` (create or see extraexamples/dakota_uq_cantilever_lhs.in)
- Determine mean system response, variability, margin to failure given (see variables section of reference manual)
  - Yield stress R ~ Normal(40000, 2000)
  - Young's modulus E ~ Normal(2.9e7, 1.45e6)
  - Horizontal load X ~ Normal(500, 100)
  - Vertical load Y ~ Normal(1000, 100)
- Hold width and thickness at 2.5
- Use `probability_levels` or `response_levels` in method
  - What is the probability(stress < 20000)?
- Extra exercises (time permitting)
  - *What happens to confidence intervals on the mean and standard deviation as number of samples varies?*
  - Instead of normal, try uniform distribution for each random variable. What do you expect would happen?

Example Input/Output: Sampling

extraexamples/dakota_uq_cantilever_lhs.in

```
method,
    sampling
      sample_type lhs
      samples = 10000   seed = 12347
      num_probability_levels = 0 17 17
      probability_levels =
      .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8 .85 .9 .95 .99 .999
       .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8 .85 .9 .95 .99 .999
      cumulative distribution

variables,
      continuous_design = 2
         initial_point 2.5 2.5
         upper_bounds 10.0 10.0
         lower_bounds 1.0 1.0
         descriptors 'beam_width' 'beam_thickness'
      normal_uncertain = 4
         means = 40000. 29.E+6 500. 1000.
         std_deviations = 2000. 1.45E+6 100. 100.
         descriptors = 'R' 'E' 'X' 'Y'

responses,
      num_response_functions = 3
      no_gradients
      no_hessians
```

Input (extra_examples/dakota_uq_cantilever_lhs.in)

Output

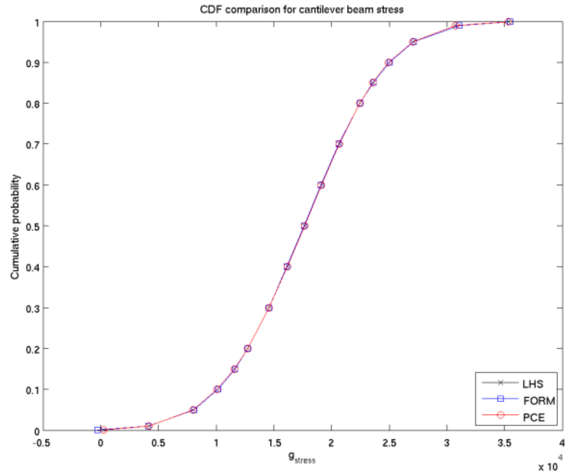
Typical UQ Output

- **Moments and confidence intervals**

```
Statistics based on 10000 samples:

Moment-based statistics for each response function:
                            Mean           Std Dev          Skewness          Kurtosis
          area  6.2500000000e+00  0.0000000000e+00              -nan              -nan
      g_stress  1.7599759864e+04  5.7886440706e+03 -2.2153567379e-02 -4.9234550018e-02
       g_displ  1.7201261575e+00  4.0670385498e-01  1.7796424852e-01  8.0009704624e-02

95% confidence intervals for each response function:
                    LowerCI_Mean      UpperCI_Mean    LowerCI_StdDev    UpperCI_StdDev
          area  6.2500000000e+00  6.2500000000e+00  0.0000000000e+00  0.0000000000e+00
      g_stress  1.7486290789e+04  1.7713228938e+04  5.7095204696e+03  5.8700072185e+03
       g_displ  1.7121539434e+00  1.7280983716e+00  4.0114471657e-01  4.1242034152e-01
```

- **CDF (and PDF) data**

```
Level mappings for each response function:
Cumulative Distribution Function (CDF) for g_stress:
     Response Level  Probability Level  Reliability Index
     --------------  -----------------  -----------------
   2.4921421856e+02   1.0000000000e-03
   4.1489075797e+03   1.0000000000e-02
   7.9708753041e+03   5.0000000000e-02
   1.0090342657e+04   1.0000000000e-01
   1.1589780322e+04   1.5000000000e-01
   1.2731567123e+04   2.0000000000e-01
   1.4564078343e+04   3.0000000000e-01
   ...
```



Adapt the Study

- What needs to change in the input to perform a polynomial chaos study?
- A local reliability analysis?
- What changes in the output?

Changes for Reliability, PCE

```
method,
      local_reliability
        mpp_search no_approx
        num_probability_levels = 0 17 17

        probability_levels =
       .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8
.85 .9 .95 .99 .999
       .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8
.85 .9 .95 .99 .999
        cumulative distribution


responses,
      descriptors = 'area' 'g_stress' 'g_displ'
      num_response_functions = 3
      analytic gradients
      no_hessians
```

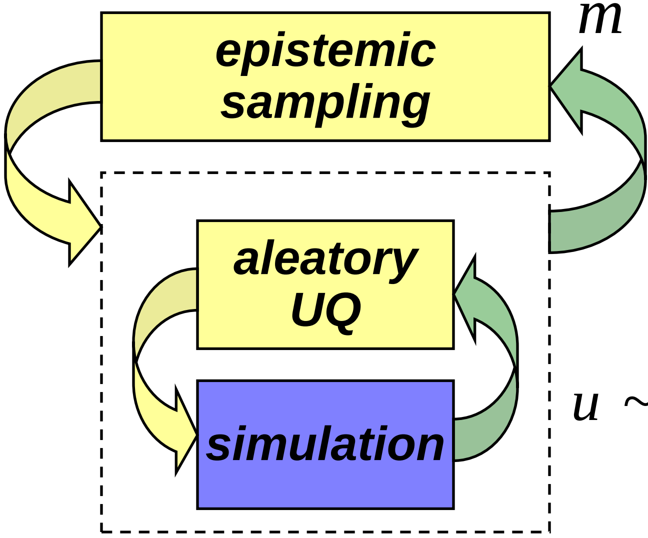
```
method,
      polynomial_chaos
        sparse_grid_level = 2 #non_nested
        sample_type lhs seed = 12347
        samples = 10000
        num_probability_levels = 0 17 17

        probability_levels =
       .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8
.85 .9 .95 .99 .999
       .001 .01 .05 .1 .15 .2 .3 .4 .5 .6 .7 .8
.85 .9 .95 .99 .999
        cumulative distribution
```

Reliability Input (examples/methods/dakota_uq_reliability.in)

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

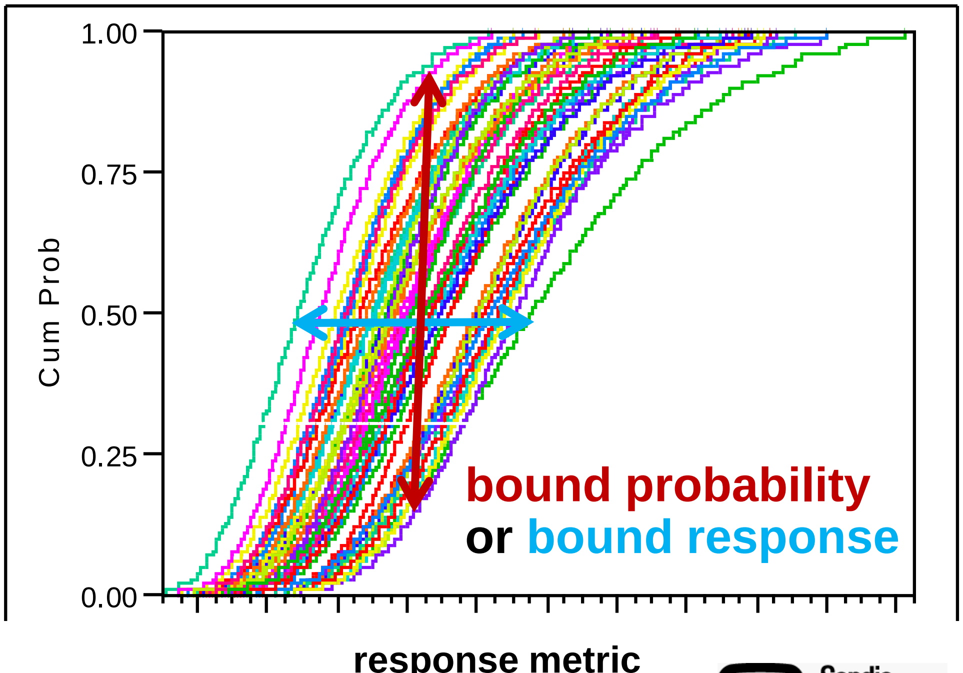
- Propagate over epistemic and aleatory uncertainty, e.g., UQ with bounds on the mean of a normal distribution (hyper-parameters)
- Typical in regulatory analyses (e.g., NRC, WIPP)
- Outer loop: epistemic (interval) variables, inner loop UQ over aleatory (probability) variables; *potentially costly,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

50 outer loop samples:
50 aleatory CDF traces



$$m \in [L, U]$$

$$u \sim N(m, \sigma)$$



“Envelope” of CDF traces represents response epistemic uncertainty

DAKOTA UQ Summary and Relevant Methods

- **What? Understand code output uncertainty / variability**
- **Why? Risk-informed decisions with variability, possible outcomes**
- **How? What DAKOTA methods are relevant?**

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

- **See DAKOTA Usage Guidelines in User's Manual**
- **Analyze tabular output with third-party statistics package**

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

Learning Goals Revisited: Uncertainty Quantification

- **Understand why you need to consider uncertainties in modeling and simulation**
- **Explain how UQ works, and what data and choices are required to perform it**
- **Be able to enumerate uncertainties in your domain and ways uncertainty-endowed code predictions could help decision making**
- **Create DAKOTA studies to perform UQ (sampling, reliability, stochastic expansions, epistemic)**
- **Understand DAKOTA statistics outputs and margin assessment**
- **How to choose from UQ options in DAKOTA for your problem**

- ***Reassess UQ relevance in your application domain***
- ***What methods, results would most help for your UQ problems?***

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