DAKOTA 101

Uncertainty Quantification

http://dakota.sandia.gov

Learning goals:

- **Motivation and definition of UQ: know when and why to apply it**
- **Brief survey of core UQ methods:**
  sampling, reliability, stochastic expansions, epistemic/mixed UQ
- **Run simple example studies**
- **Understand options for post-processing the output uncertainty**

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Risk-informed Decision Making, QMU, & UQ: An ASC V&V Program Perspective

Labs are shifting from test-based to M&S-based design and certification.

In order to support risk-informed decision-making based on M&S, we require:

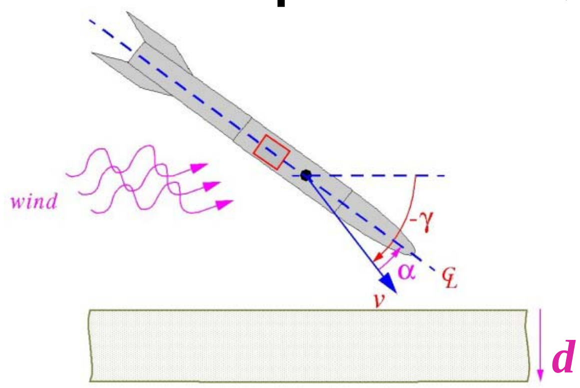
- ***Predictive simulations:*** **verified and validated for application of interest**
- ***Quantified uncertainties:*** **the effect of random variability is fully understood**

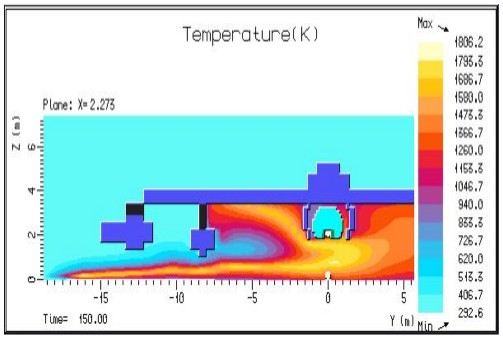
DOE process: "Quantification of Margins and Uncertainties (QMU)"

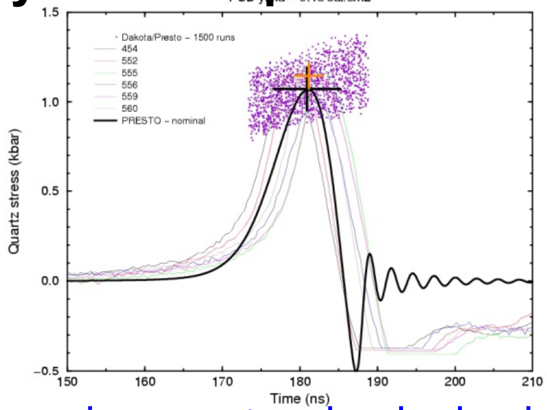
→ provide *best estimate* + *uncertainty* in the decision-making context

Uncertainty Quantification

Critical component of QMU → credible M&S capability for stockpile stewardship





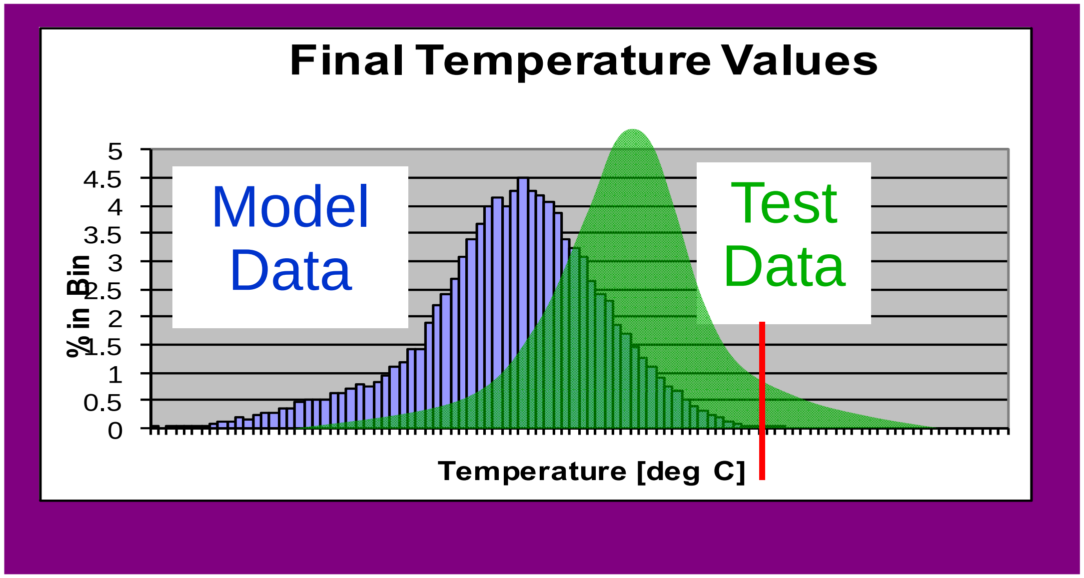


Uncertainty applications: penetration, joint mechanics, abnormal environments, shock physics, …

Uncertainties in Simulation and Validation

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!*

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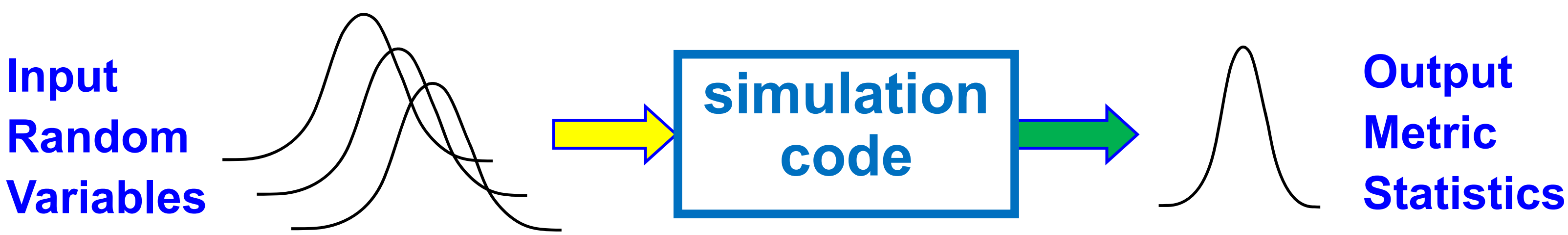
Categories of Uncertainty

Often useful algorithmic distinctions, but not always a clear division

- 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



Categories of Uncertainty

Often useful algorithmic distinctions, but not always a clear division

- 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

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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)*

(possibly given distributions)

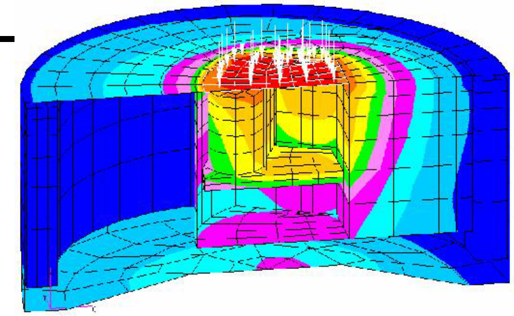
(here assumed a black-box)

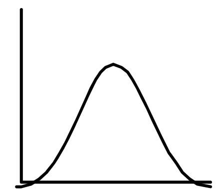
Potential Goals:

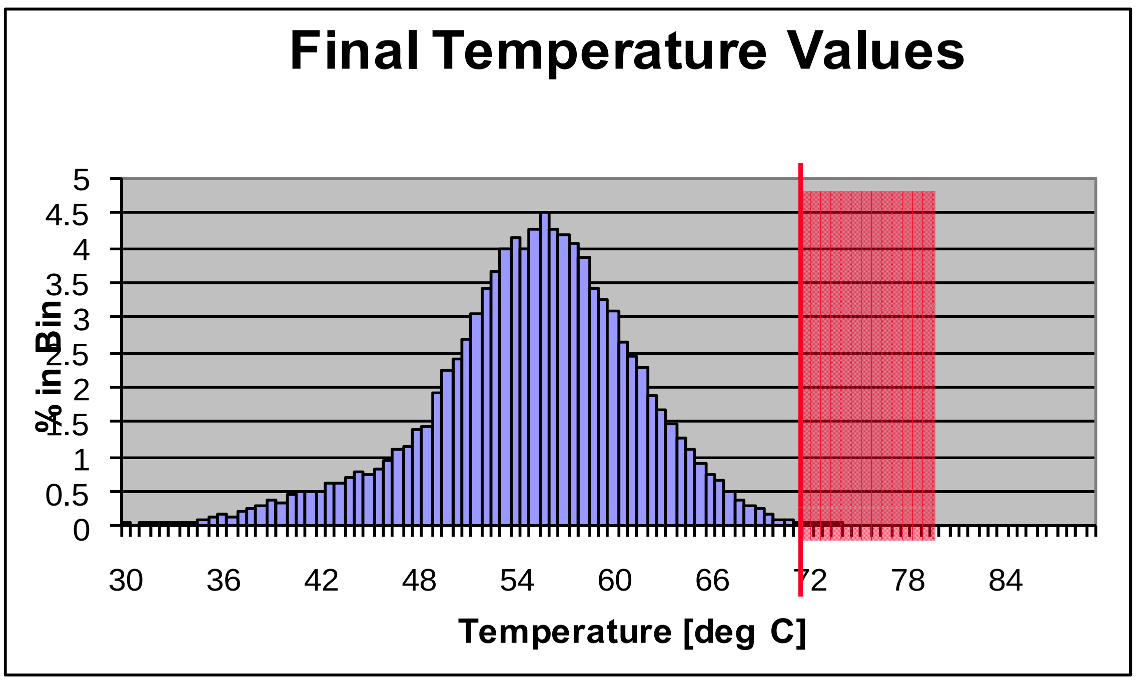
- based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)
- validation: is the model sufficient *for the intended application?*
- quantification of margins and uncertainties (QMU): *how close are uncertainty-aware code predictions to performance expectations or limits?*
- *quantify uncertainty when using calibrated model to predict*

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*

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Uncertainty Quantification Algorithms @ SNL: New methods bridge robustness/efficiency gap

	Production	New	Under dev.	Planned	Collabs.
Sampling	Latin Hypercube, Monte Carlo	Importance, Incremental		Bootstrap, Jackknife	FSU
Reliability	*Local:* Mean Value, First-order & second-order reliability methods (FORM, SORM)	*Global:* Efficient global reliability analysis (EGRA)	gradient-enhanced	Ensemble emulator-based	*Local:* Notre Dame, *Global:* Vanderbilt
Stochastic expansion		Polynomial chaos expansion, Stochastic collocation	Dimension-adaptive p-/h-refinement, gradient-enhanced	Region-adaptive, discrete, multi-physics	Stanford, Purdue, Austr. Natl., FSU
Other probabilistic		Random fields/ stochastic proc.		Dimension reduction	Cornell, Maryland
Epistemic	Interval-valued/ Second-order prob. (nested sampling)	Opt-based interval estimation, Dempster-Shafer	Bayesian	Imprecise probability	LANL, Applied Biometrics
Metrics & Global SA	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		UNM

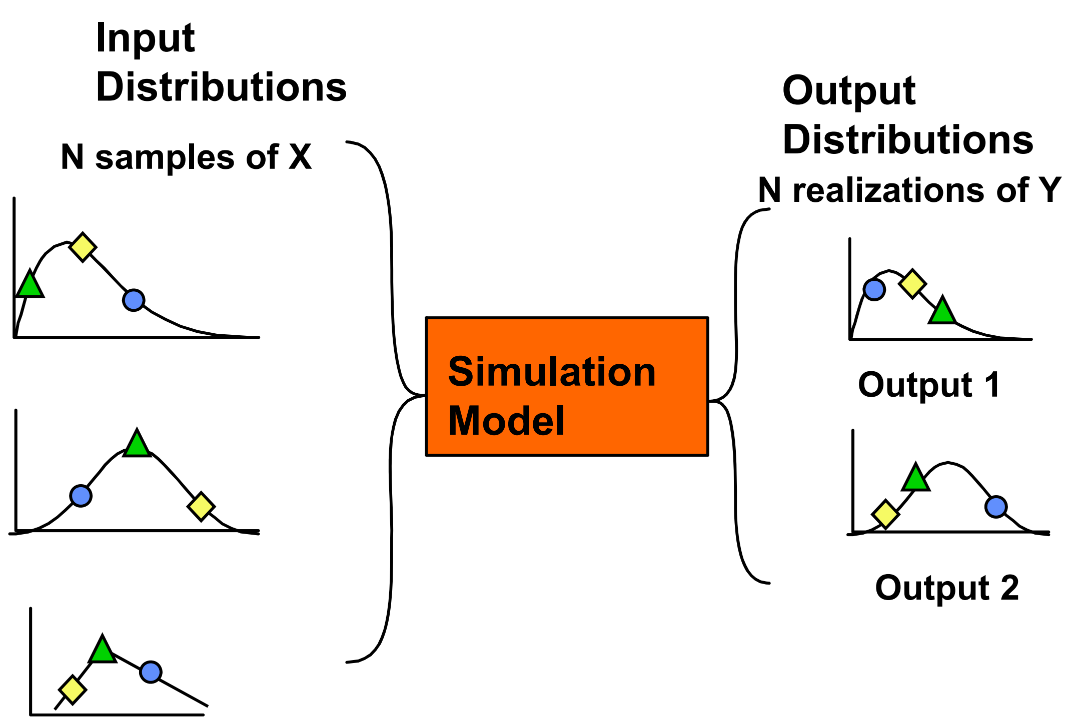
Reseach: Tailoring & Adaptivity

Adv. Deployment

Fills Gaps

Common 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



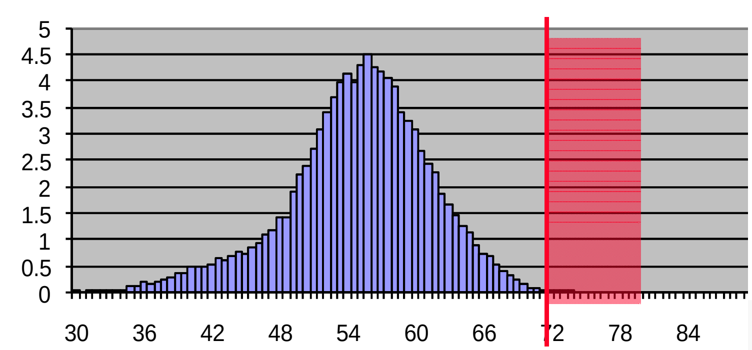
- sample mean

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

- sample variance

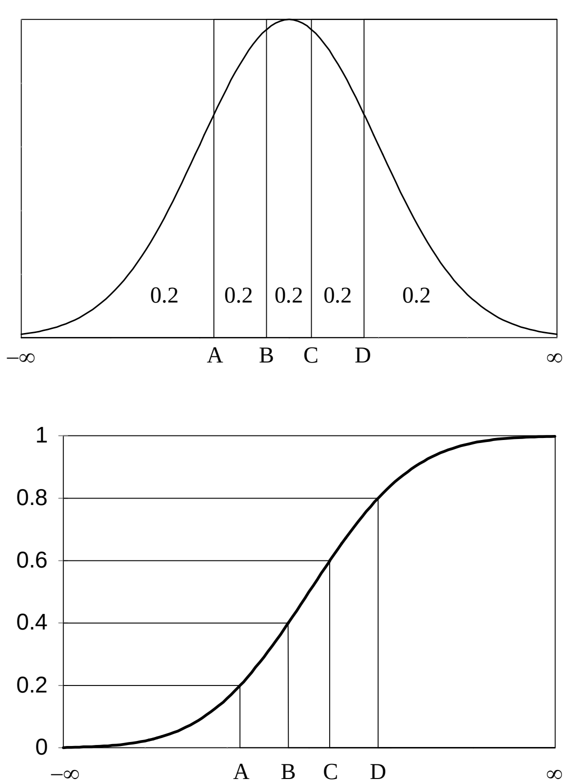
$$T_{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}\left[T(u^i) - \bar{T}\right]^2$$

- full PDF(probabilities)



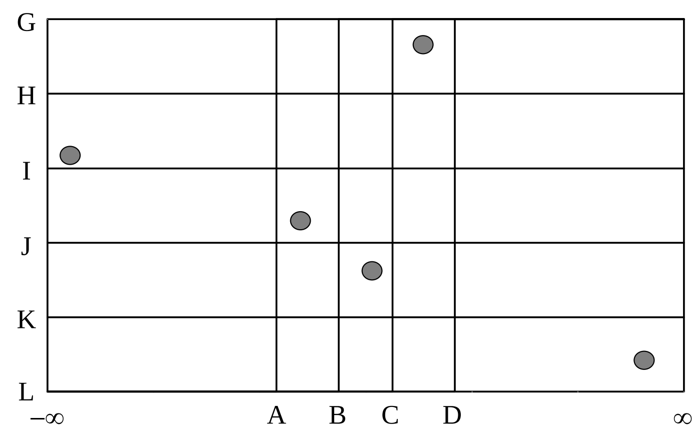
Latin Hypercube Sampling

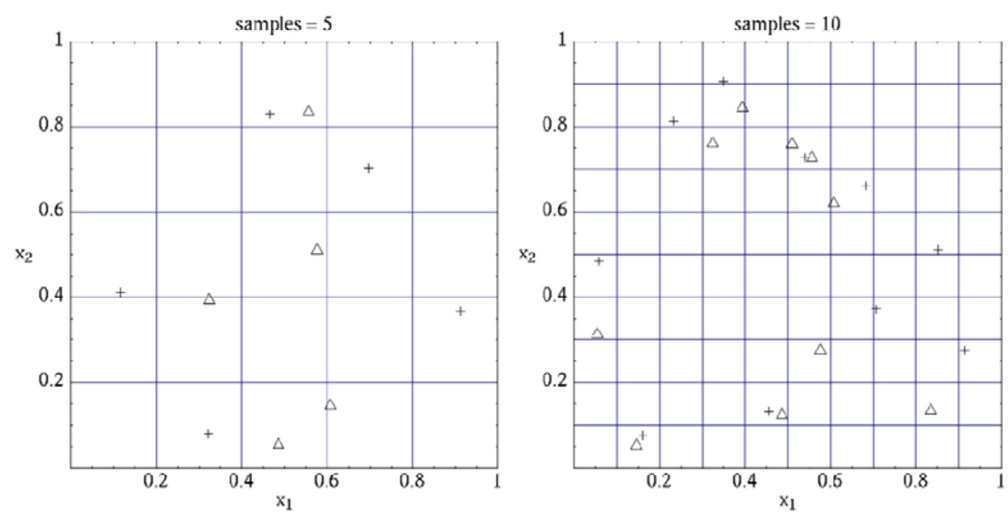
- **LHS is stratified random sampling among equal probability bins for all 1-D projections of an n-dimensional set of samples.**
  - **Early work by McKay and Conover**
  - **Restricted pairing by Iman → enforce prescribed input correlations**



Intervals Used with a LHS of Size N = 5 in Terms of the PDF and CDF for a Normal Random Variable

A possible LHS for n=2, N=5 with X1 = normal and X2 = uniform





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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

```
strategy
      single_method graphics

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
#      output silent

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'

interface,
      direct analysis_driver = 'mod_cantilever'

responses,
      num_response_functions = 3
      no_gradients
      no_hessians
```

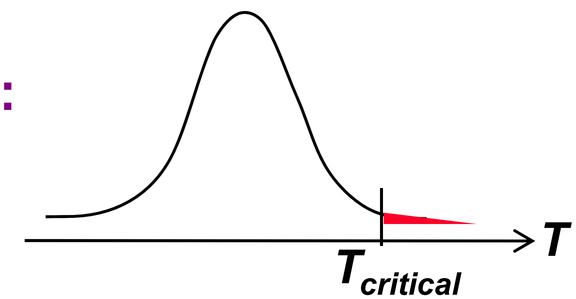
Input (extra_examples/dakota_uq_cantilever_lhs.in)

```
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

Level mappings for each response function:
Cumulative Distribution Function (CDF) for g_stress:
     Response Level  Probability Level  Reliability Index  General Rel 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
   1.6151010310e+04   4.0000000000e-01
   1.7689441098e+04   5.0000000000e-01
   1.9129203866e+04   6.0000000000e-01
   2.0683233939e+04   7.0000000000e-01
   2.2457356004e+04   8.0000000000e-01
   2.3589089220e+04   8.5000000000e-01
   2.4920875151e+04   9.0000000000e-01
   2.7044322788e+04   9.5000000000e-01
   3.0752664401e+04   9.9000000000e-01
   3.5331778223e+04   9.9900000000e-01
Cumulative Distribution Function (CDF) for g_displ:
     Response Level  Probability Level  Reliability Index  General Rel Index
     --------------  -----------------  -----------------  -----------------
   5.8671224313e-01   1.0000000000e-03
   8.3043198982e-01   1.0000000000e-02
   1.0603181923e+00   5.0000000000e-02
   1.2097669707e+00   1.0000000000e-01
   1.2966885568e+00   1.5000000000e-01
   1.3746930033e+00   2.0000000000e-01
   1.5000347941e+00   3.0000000000e-01
   1.6076526708e+00   4.0000000000e-01
   1.7093341472e+00   5.0000000000e-01
   1.8116530545e+00   6.0000000000e-01
   1.9242640620e+00   7.0000000000e-01
   2.0601011526e+00   8.0000000000e-01
   2.1419095361e+00   8.5000000000e-01
   2.2454142842e+00   9.0000000000e-01
   2.3966062187e+00   9.5000000000e-01
   2.7299039059e+00   9.9000000000e-01
   3.0858487193e+00   9.9900000000e-01
```

Output

Challenge: 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**

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

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

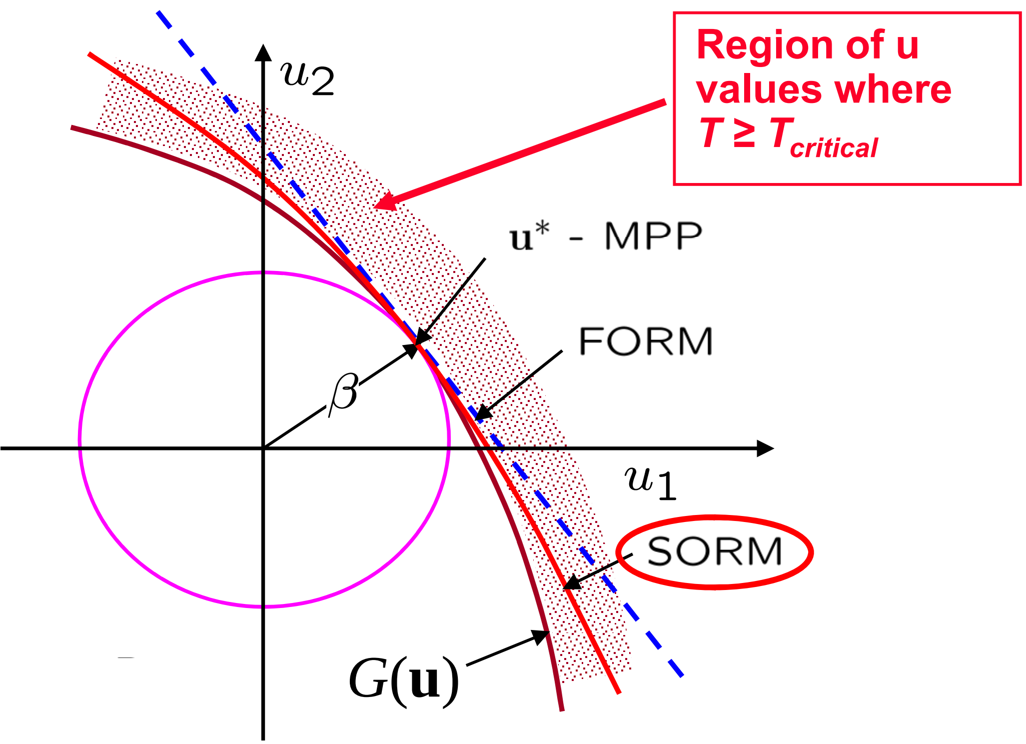
All the usual nonlinear optimization tricks apply…

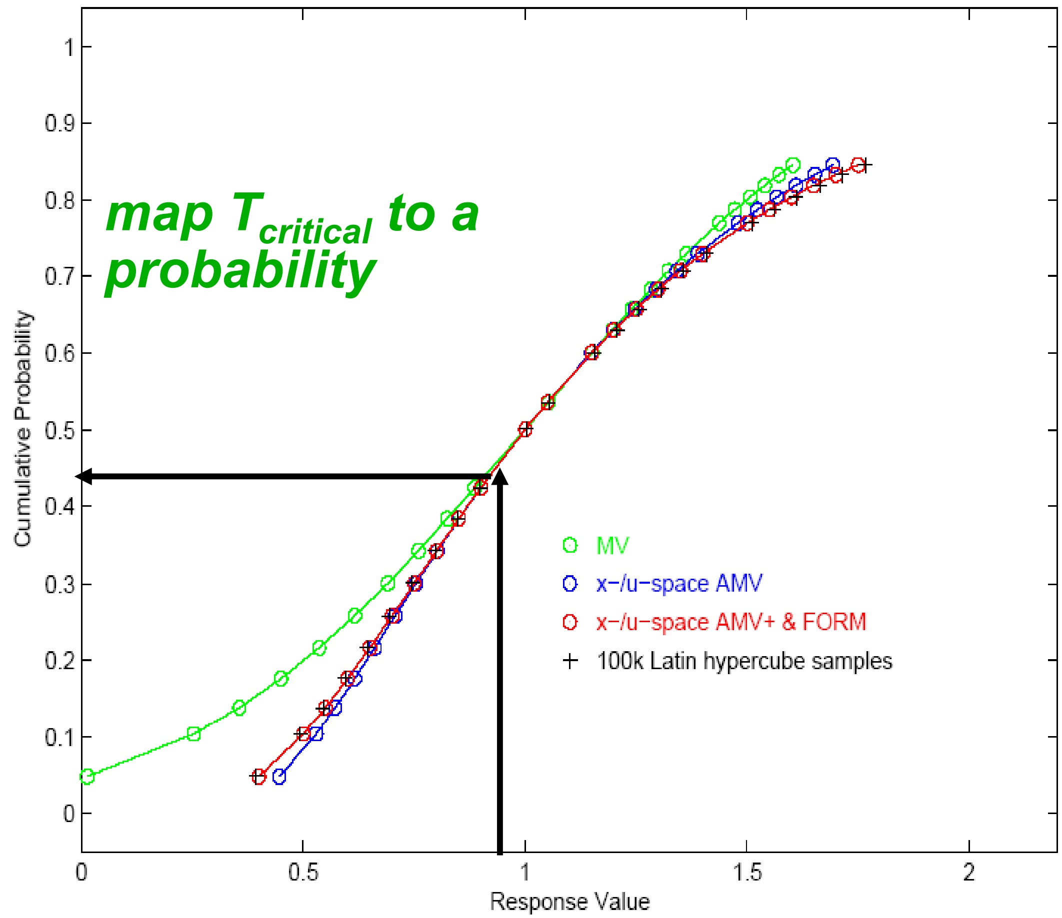
Analytic Reliability: MPP Search

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)

$$\begin{array}{ll} \text{minimize} & \mathbf{u}^T\mathbf{u} \\ \text{subject to} & G(\mathbf{u}) = \bar{z} \end{array}$$

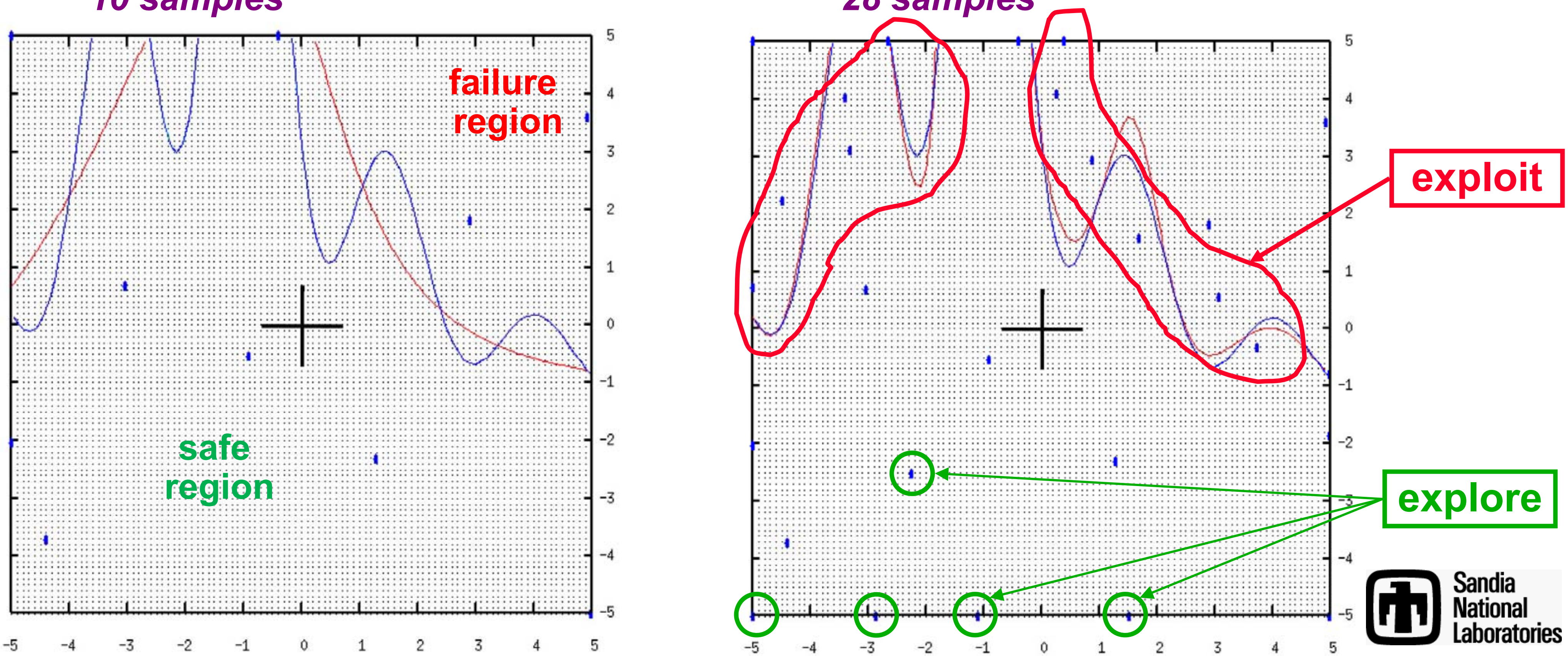




Efficient Global Reliability Analysis: GP Surrogate + MMAIS (B.J. Bichon)

- Apply an EGO-like method to the equality-constrained optimization problem
- In EGRA, an expected feasibility function balances exploration with local search near the failure boundary to refine the GP
- Cost competitive with best 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 *28 samples*



Local Reliability Example

- Compare sampling methods to local reliability methods (modify `dakota_uq_cantilever_lhs.in` or create `dakota_uq_cantilever_rel.in`)
- Use local_reliability method with mpp_search option

Example Input/Output: Reliability

```
strategy
     single_method #graphics

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

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'

interface,
     direct
       analysis_driver = 'mod_cantilever'

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

```
<<<<< Function evaluation summary: 437 total (435 new, 2 duplicate)
-----------------------------------------------------------------
Cumulative Distribution Function (CDF) for g_stress:
     Response Level  Probability Level  Reliability Index  General Rel Index
     --------------  -----------------  -----------------  -----------------
  -2.8366322206e+02   9.9999999999e-04   3.0902323062e+00   3.0902323062e+00
   4.1370568311e+03   1.0000000000e-02   2.3263478740e+00   2.3263478740e+00
   8.0809718495e+03   5.0000000000e-02   1.6448536270e+00   1.6448536270e+00
   1.0183458352e+04   1.0000000000e-01   1.2815515655e+00   1.2815515655e+00
   1.1601996014e+04   1.5000000000e-01   1.0364333895e+00   1.0364333895e+00
   1.2729404779e+04   2.0000000000e-01   8.4162123357e-01   8.4162123357e-01
   1.4565211274e+04   3.0000000000e-01   5.2440051271e-01   5.2440051271e-01
   1.6133840235e+04   4.0000000000e-01   2.5334710314e-01   2.5334710314e-01
   1.7599296043e+04   4.9995140020e-01   1.2182163305e-04   1.2182163305e-04
   1.9066159765e+04   6.0000000000e-01  -2.5334710314e-01  -2.5334710314e-01
   2.0634788726e+04   7.0000000000e-01  -5.2440051271e-01  -5.2440051271e-01
   2.2470595221e+04   8.0000000000e-01  -8.4162123357e-01  -8.4162123357e-01
   2.3598003986e+04   8.5000000000e-01  -1.0364333895e+00  -1.0364333895e+00
   2.5016541648e+04   9.0000000000e-01  -1.2815515655e+00  -1.2815515655e+00
   2.7119028150e+04   9.5000000000e-01  -1.6448536270e+00  -1.6448536270e+00
   3.1062943169e+04   9.9000000000e-01  -2.3263478740e+00  -2.3263478740e+00
   3.5483663222e+04   9.9900000000e-01  -3.0902323062e+00  -3.0902323062e+00
Cumulative Distribution Function (CDF) for g_displ:
     Response Level  Probability Level  Reliability Index  General Rel Index
     --------------  -----------------  -----------------  -----------------
   5.2190342194e-01   1.0000000000e-03   3.0902323062e+00   3.0902323062e+00
   7.9940521862e-01   1.0000000000e-02   2.3263478740e+00   2.3263478740e+00
   1.0530040474e+00   5.0000000000e-02   1.6448536270e+00   1.6448536270e+00
   1.1908432559e+00   1.0000000000e-01   1.2815515655e+00   1.2815515655e+00
   1.2849790018e+00   1.5000000000e-01   1.0364333895e+00   1.0364333895e+00
   1.3604842916e+00   2.0000000000e-01   8.4162123357e-01   8.4162123357e-01
   1.4848060107e+00   3.0000000000e-01   5.2440051271e-01   5.2440051271e-01
   1.5924532498e+00   4.0000000000e-01   2.5334710314e-01   2.5334710314e-01
   1.6943072241e+00   4.9999077279e-01   2.3129179837e-05   2.3129179837e-05
   1.7974470361e+00   6.0000000000e-01  -2.5334710314e-01  -2.5334710314e-01
   1.9092590248e+00   7.0000000000e-01  -5.2440051271e-01  -5.2440051271e-01
   2.0421553573e+00   8.0000000000e-01  -8.4162123357e-01  -8.4162123357e-01
   2.1249148356e+00   8.5000000000e-01  -1.0364333895e+00  -1.0364333895e+00
   2.2303425020e+00   9.0000000000e-01  -1.2815515655e+00  -1.2815515655e+00
   2.3893977168e+00   9.5000000000e-01  -1.6448536270e+00  -1.6448536270e+00
   2.6975188966e+00   9.9000000000e-01  -2.3263478740e+00  -2.3263478740e+00
   3.0598390500e+00   9.9900000000e-01  -3.0902323062e+00  -3.0902323062e+00
```

Reliability Input (examples/methods/dakota_uq_reliability.in)

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(ξ) ≈ f(u)

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

- **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)**

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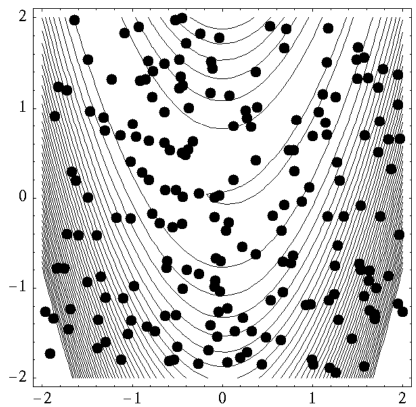
Forming PCE/SC Expansions (for PCE, using R^i to estimate α_j)

Random sampling: PCE

Expectation (sampling):
- Sample w/i distribution of x
- Compute expected value of product of R and each Y_j

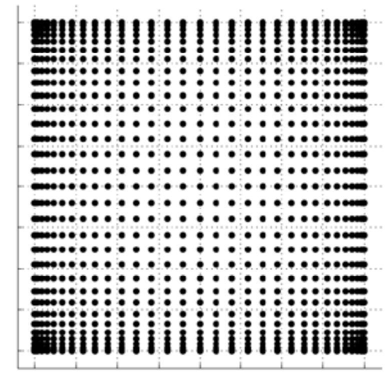
Linear regression ("point collocation"):

$$\boxed{\Psi\alpha = R}$$

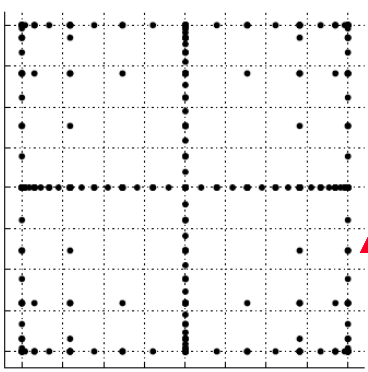


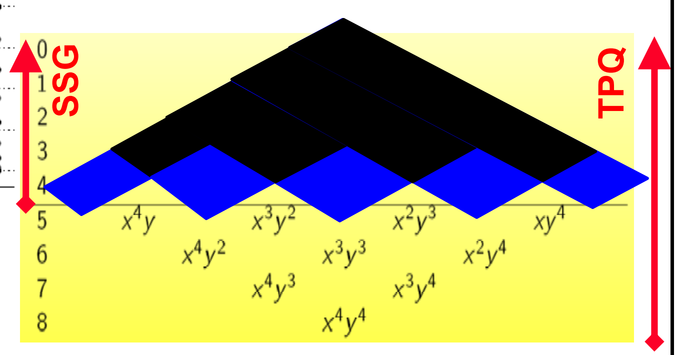
Tensor-product quadrature: PCE/SC

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



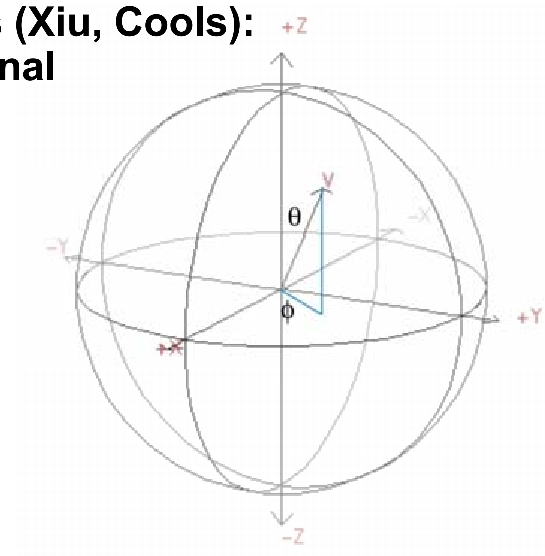
Smolyak Sparse Grid: PCE/SC





Cubature: PCE

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



Stochastic Expansion Example

- **Compare PCE to sampling and local reliability methods (modify `dakota_cantilever_lhs.in` or `dakota_cantilever_rel.in`)**

Example Input/Output: PCE

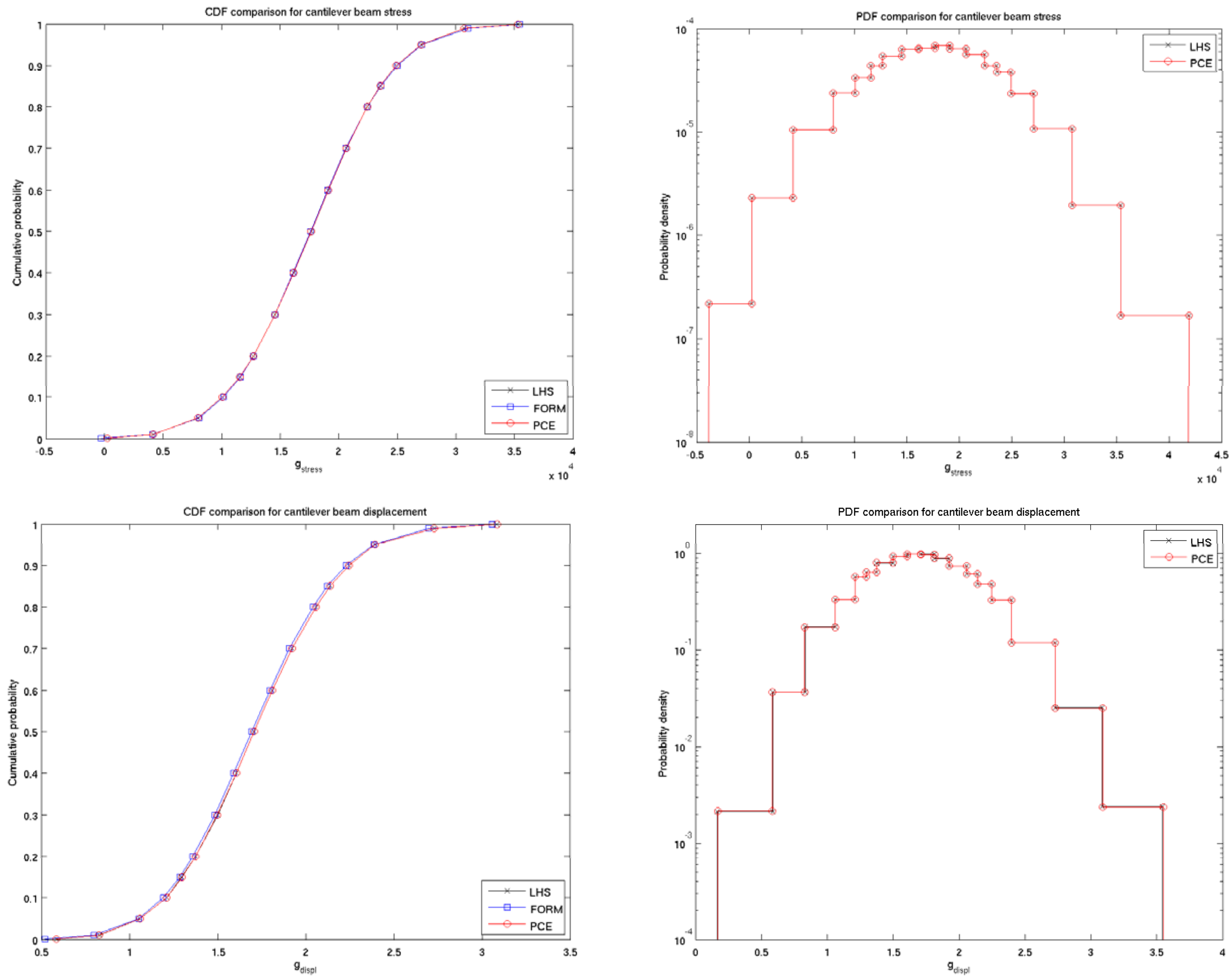
Input (extra_examples/dakota_uq_cantilever_pce.in)

```
strategy
     single_method graphics

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
#      output silent

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'

interface,
     direct
       analysis_driver = 'mod_cantilever'

responses,
     descriptors = 'area' 'g_stress' 'g_displ'
     num_response_functions = 3
     no_gradients
     no_hessianse
```

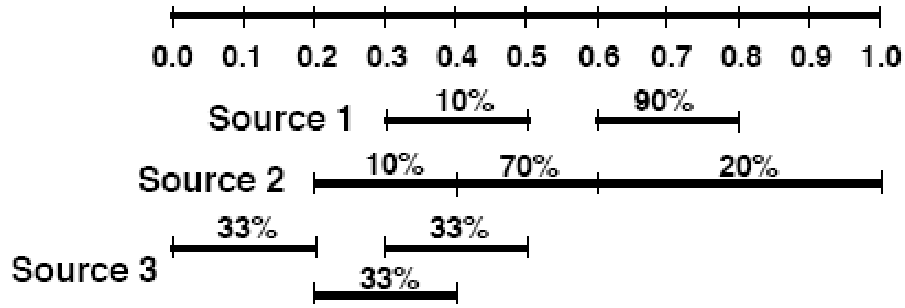
Output

```
<<<<< Function evaluation summary: 57 total (57 new, 0 duplicate)
-------------------------------------------------------------------
Polynomial Chaos coefficients for area:
        coefficient   u1   u2   u3   u4
        ----------- ---- ---- ---- ----
   6.2500000000e+00  He0  He0  He0  He0   ...
Polynomial Chaos coefficients for g_stress:
        coefficient   u1   u2   u3   u4
        ----------- ---- ---- ---- ----
   1.7600000000e+04  He0  He0  He0  He0 ...
Polynomial Chaos coefficients for g_displ:
        coefficient   u1   u2   u3   u4
        ----------- ---- ---- ---- ----
   1.7201243431e+00  He0  He0  He0  He0 ...

Statistics derived analytically from polynomial expansion:

Moment-based statistics for each response function:
                            Mean           Std Dev          Skewness          Kurtosis
area
  expansion:    6.2500000000e+00  2.4824701829e-15
  numerical:    6.2500000000e+00  7.1054273576e-15  1.0000000000e+00 -2.0000000000e+00
g_stress
  expansion:    1.7600000000e+04  5.7871581973e+03
  numerical:    1.7600000000e+04  5.7871581973e+03  9.4100742175e-15  6.2172489379e-15
g_displ
  expansion:    1.7201243431e+00  4.0644795983e-01
  numerical:    1.7201243431e+00  4.0644787032e-01  1.5009952217e-01  4.9005496977e-02

Statistics based on 10000 samples performed on polynomial expansion:

Cumulative Distribution Function (CDF) for g_stress:
     Response Level  Probability Level  Reliability Index  General Rel Index
     --------------  -----------------  -----------------  -----------------
   2.4921421856e+02   1.0000000000e-03
   4.1489075797e+03   1.0000000000e-02
   ...
   3.0752664401e+04   9.9000000000e-01
   3.5331778223e+04   9.9900000000e-01
Cumulative Distribution Function (CDF) for g_displ:
     Response Level  Probability Level  Reliability Index  General Rel Index
     --------------  -----------------  -----------------  -----------------
   5.8392829293e-01   1.0000000000e-03
   8.2796204947e-01   1.0000000000e-02
   ...
   2.7290918315e+00   9.9000000000e-01
   3.0882954345e+00   9.9900000000e-01
```

Comparison of Sampling, Reliability, PCE

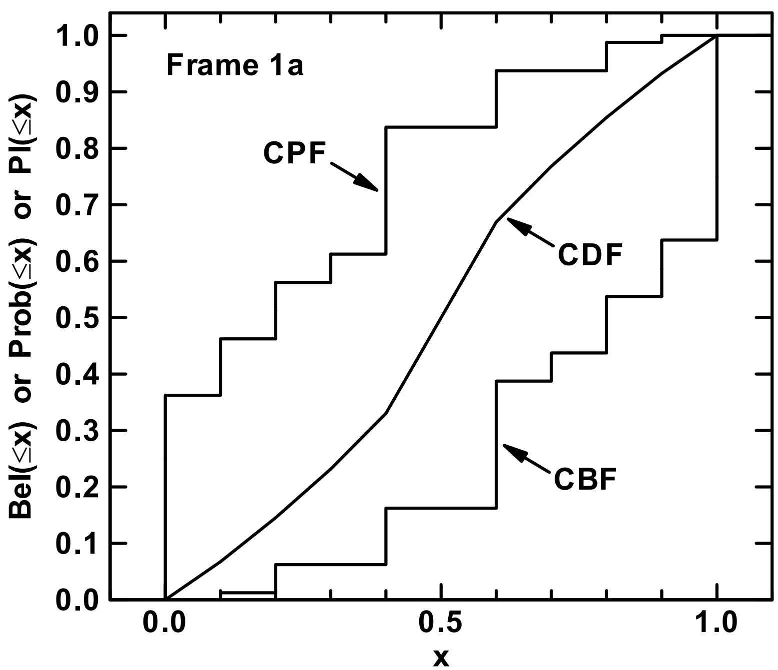


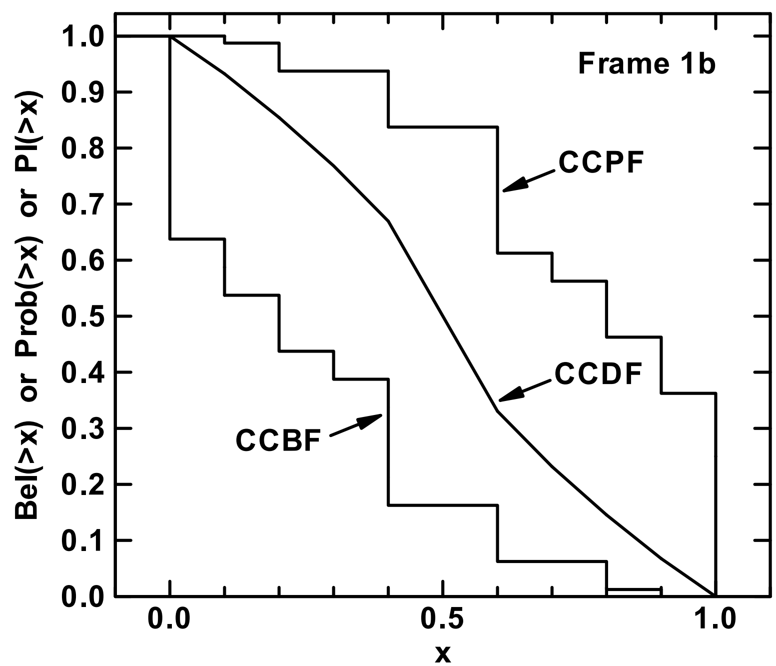
Epistemic UQ: Dempster-Shafer Theory



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.





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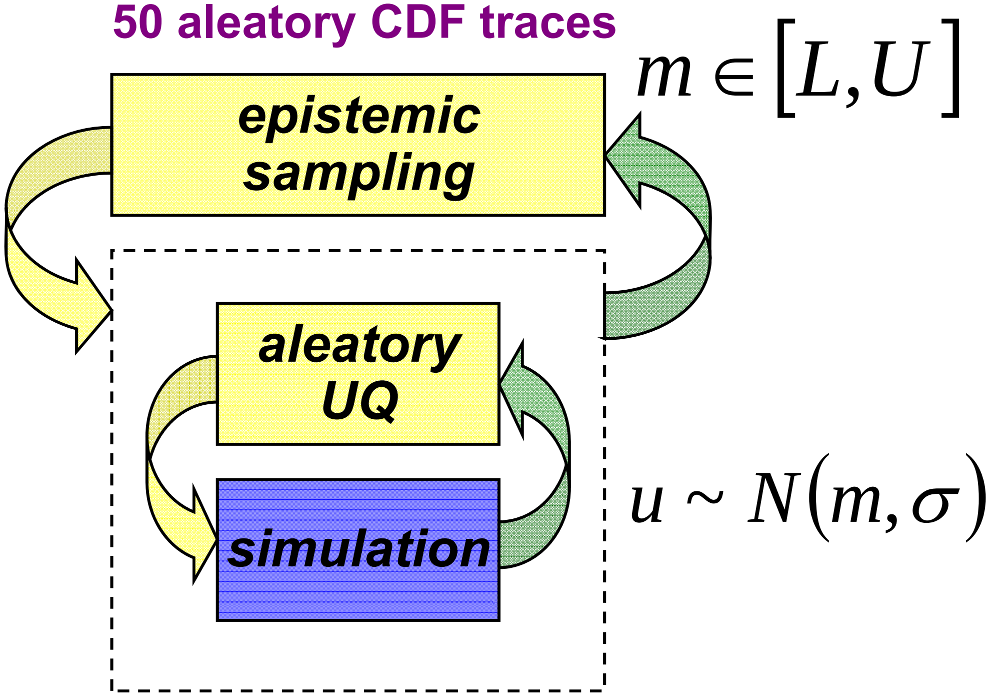
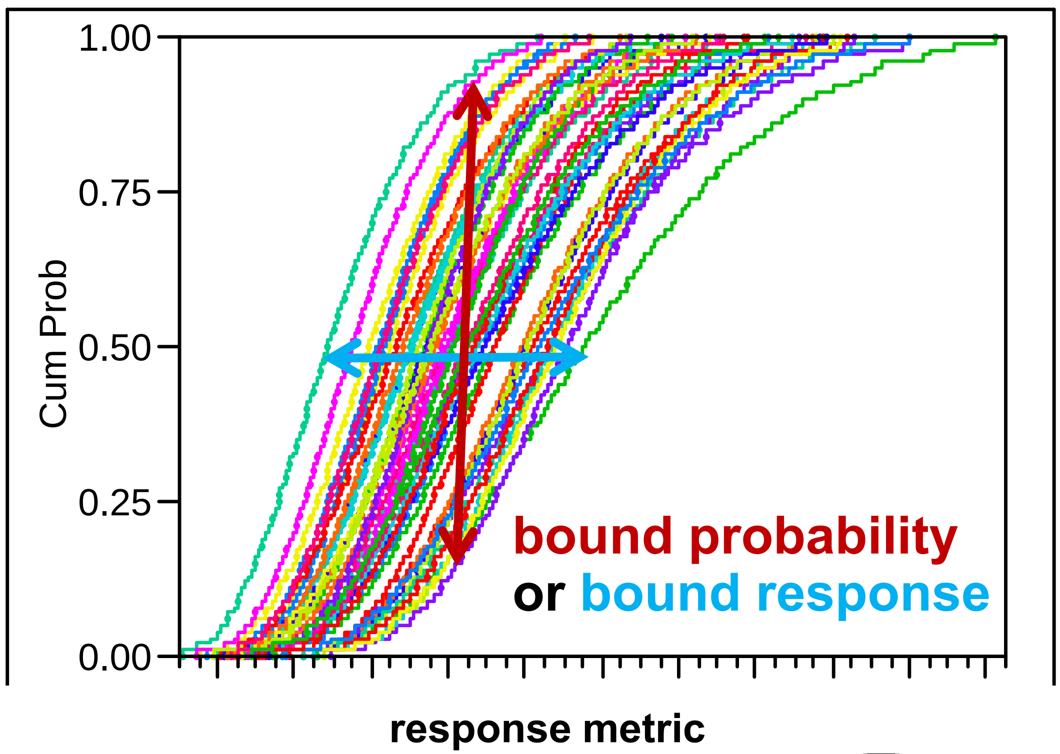
Epistemic UQ: Nested ("Second-order")Approaches

- **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





"Envelope" of CDF traces represents response epistemic uncertainty

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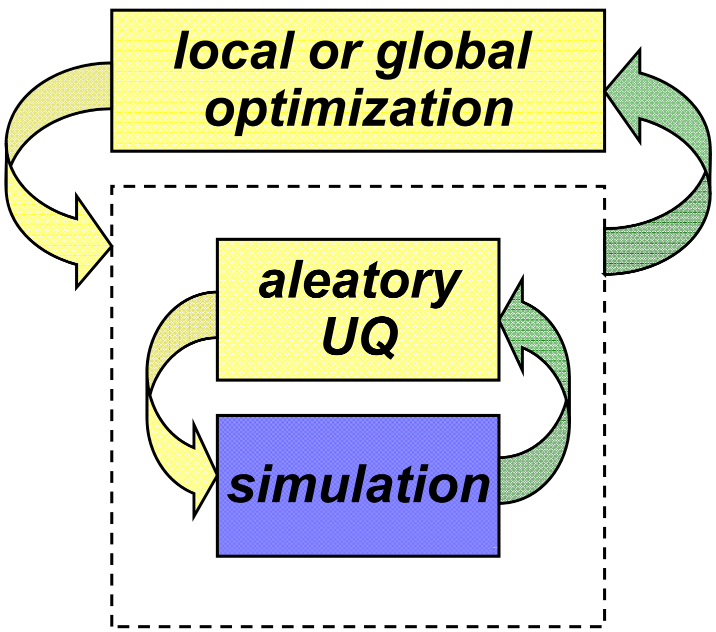
Interval Estimation Approach (Probability Bounds Analysis)



- *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

$$\min_{u_E} \; f_{STAT}(u_A \mid u_E)$$
$$u_{LB} \le u_E \le u_{UB}$$
$$u_A \sim F(u_A; u_E)$$

$$\max_{u_E} \; f_{STAT}(u_A \mid u_E)$$
$$u_{LB} \le u_E \le u_{UB}$$
$$u_A \sim F(u_A; u_E)$$

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DAKOTA UQ

- **Techniques for propagating aleatory uncertainty (variables characterized by probability distributions) through models:**
  - Latin hypercube (and other) sampling
  - Local reliability methods (mean value, MPP search, FORM, SORM)
  - Global reliability methods (EGRA)
  - Non-intrusive stochastic expansion methods (polynomial chaos and stochastic collocation)
  - *Reliability and importance sampling help with low probability events*
- **Methods for epistemic uncertainty (variables characterized by intervals or basic probability assignments):**
  - Local/global interval estimation
  - Local/global Dempster-Shafer evidence theory (belief/plausibility)
  - "Second-order" probability via sampling

- **DAKOTA can output moments, probability of response thresholds, reliability metrics, response corresponding to a metric, etc.**

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