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Aleatory and Epistemic Uncertainty Quantification for Engineering Applications

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Engineering Applications Motivation

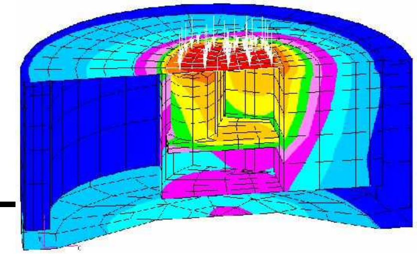
- Most computer models for engineering applications are developed to help assess a design or regulatory requirement.
- The capability to quantify the impact of variability and uncertainty in the decision context is critical, e.g.

  Prob(System Response > T) < 0.01
- This presentation discusses 5 uncertainty quantification (UQ) methods.
  - Latin Hypercube sampling
  - Analytic reliability methods
  - Polynomial chaos expansions
  - Dempster-Shafer theory of evidence
  - "Second-order" probability analysis
- These methods are all implemented in DAKOTA

Uncertainty Quantification Methods

- Goals of UQ methods:
  - Based on uncertain inputs (UQ), determine distribution function of outputs and probabilities of failure (reliability metrics)
  - Quantify the effect that uncertain (nondeterministic) input variables have on model output
  - Identify parameter correlations/local sensitivities, robust optima
  - Identify inputs whose variances contribute most to output variance (global sensitivity analysis)
  - Epistemic sensitivity analysis studies when the uncertain parameters only have bounds (intervals)

DAKOTA Overview



iterative analysis…

DAKOTA
optimization, uncertainty quant, parameter est., sensitivity analysis

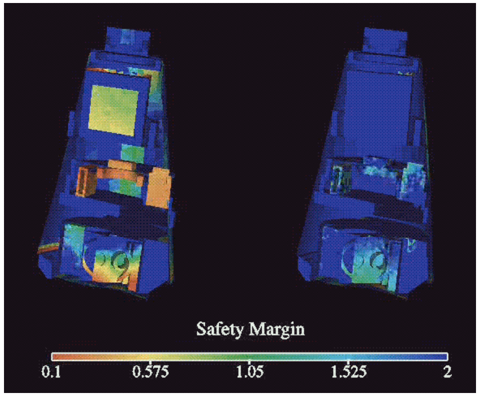
parameters
(design, UC, state)

response metrics

Computational Model
- Black box: Sandia or commercial simulation codes
- Semi-intrusive: SIERRA multi-physics, SALINAS, Xyce, Matlab, ModelCenter

Goal: answer fundamental engineering questions
- What is the best design? How safe is it?
- How much confidence do I have in my answer?

Challenges
- **Software:** reuse tools and common interfaces
- **Algorithm R&D:** nonsmooth/discontinuous/multimodal, mixed variables, unreliable gradients, costly sim. failures
- **Scalable parallelism:** ASCI-scale apps & architectures



Nominal Optimized

Impact: Tool for DOE labs and external partners, broad application deployment, free via GNU GPL (~3000 download registrations)

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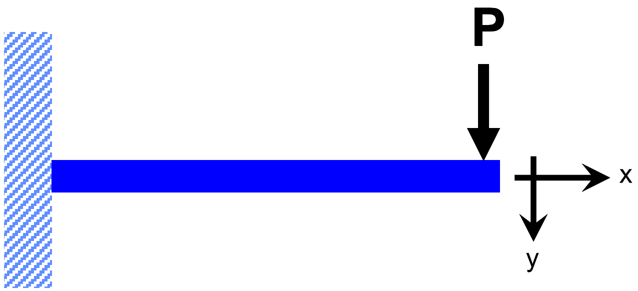
Cantilever Beam Description



- **Goal: understand how the deflection of the beam varies with respect to the length, width, and height of the beam as well as to applied load and elastic modulus of the beam**

Variable	Description	Nominal Value
L	Length	1 m
W	Width	1 cm
H	Height	2 cm
I	Area Moment of Inertia	$1/12\ WH^3$
P	Load	100 N
E	Elastic Modulus of Aluminum 6061-T6	69 GPa

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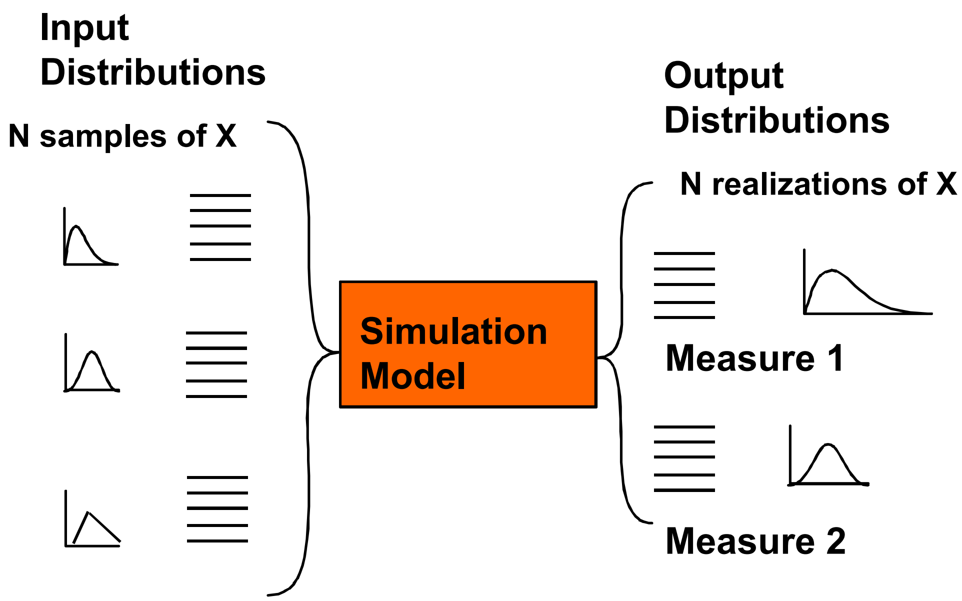
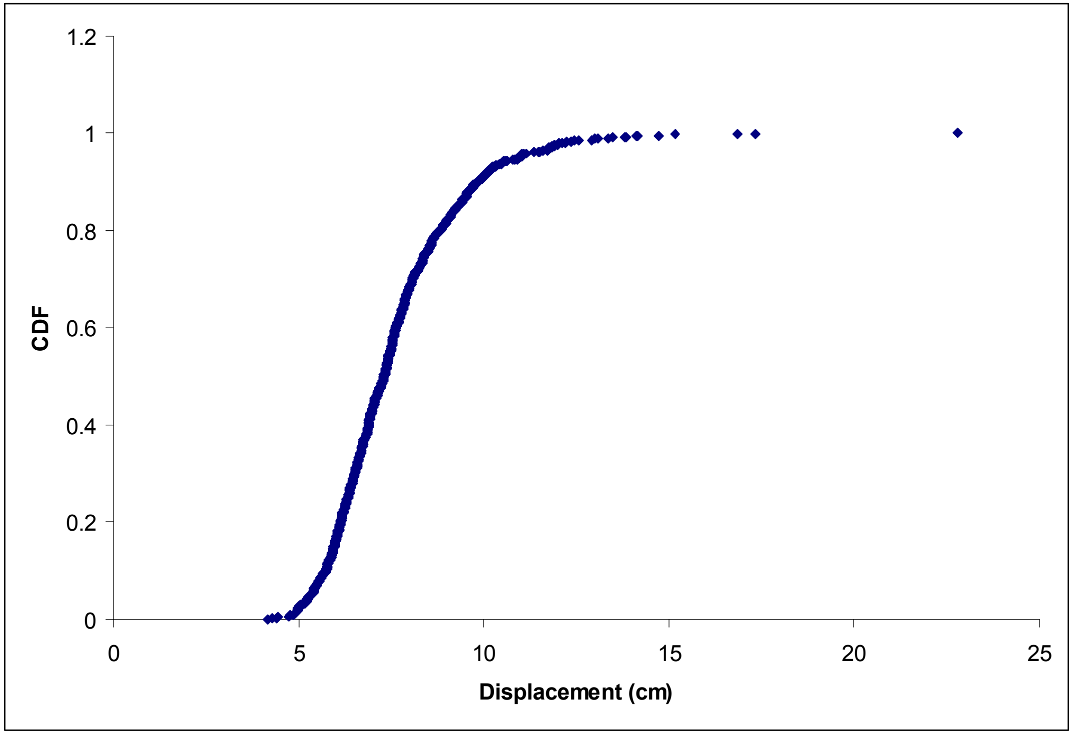
Sampling

- Much work has been done to develop efficient methods of Monte Carlo sampling, including stratified sampling (Latin hypercube sampling) which spread the samples over the space, or quasi-Monte Carlo sampling
- Sampling is not the most efficient UQ method, but it is easy to implement and is transparent in terms of tracing sample realizations through multiple codes for complex UQ studies

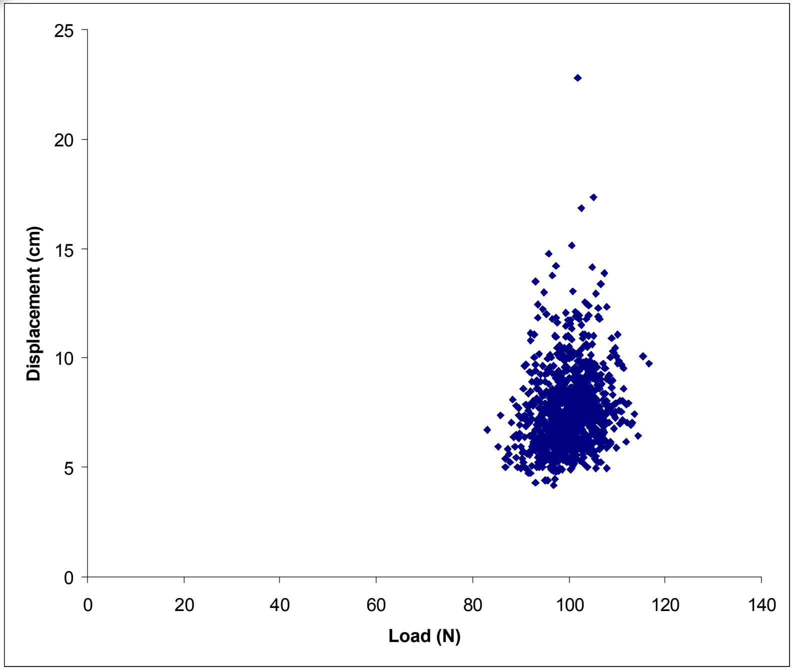


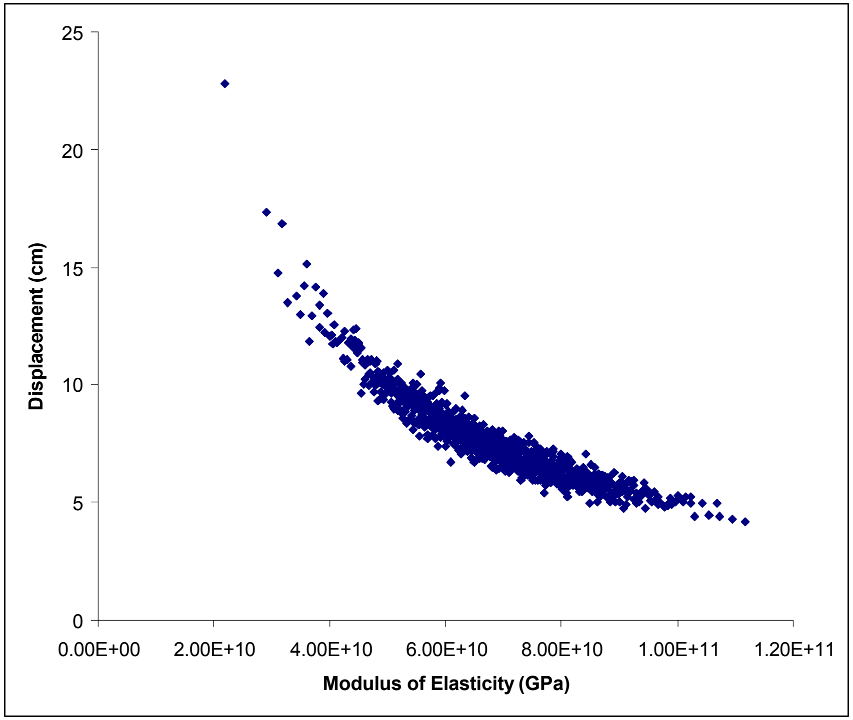
Sampling Results

Variable	Distribution	Distribution Parameters
L	Normal	Mean = 1m Std. Dev. = 0.01 m
W	Fixed	1 cm
H	Fixed	2 cm
P	Normal	Mean = 100 N Std. Dev. = 5 N
E	Normal	Mean = 69 GPa Std. Dev. = 13.8 GPa



Sampling Results





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Analytic Reliability Methods

- Define limit state function *g(x)* for response metric (model output, e.g., F_{min}) of interest, where x are uncertain variables.
- Reliability methods either
  - map specified response levels $g(x) = \bar{z}$ (perhaps corr. to a failure condition) to reliability index ***β*** or probability p; or
  - map specified probability or reliability levels to the corresponding response levels.

<u>**Mean Value (first order, second moment – MVFOSM)**</u>

determine mean and variance of limit state, translate to from p, β:

$$\mu_g = g(\mu_{\mathbf{x}})$$

$$\sigma_g = \sum_i \sum_j Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}})$$

$$\bar{z} \rightarrow p, \beta \begin{cases} \beta_{cdf} = \dfrac{\mu_g - \bar{z}}{\sigma_g} \\ \beta_{ccdf} = \dfrac{\bar{z} - \mu_g}{\sigma_g} \end{cases} \qquad \bar{p}, \bar{\beta} \rightarrow z \begin{cases} z = \mu_g - \sigma_g \bar{\beta}_{cdf} \\ z = \mu_g + \sigma_g \bar{\beta}_{ccdf} \end{cases}$$

simple approx., but widely used by analysts; also second order formulations

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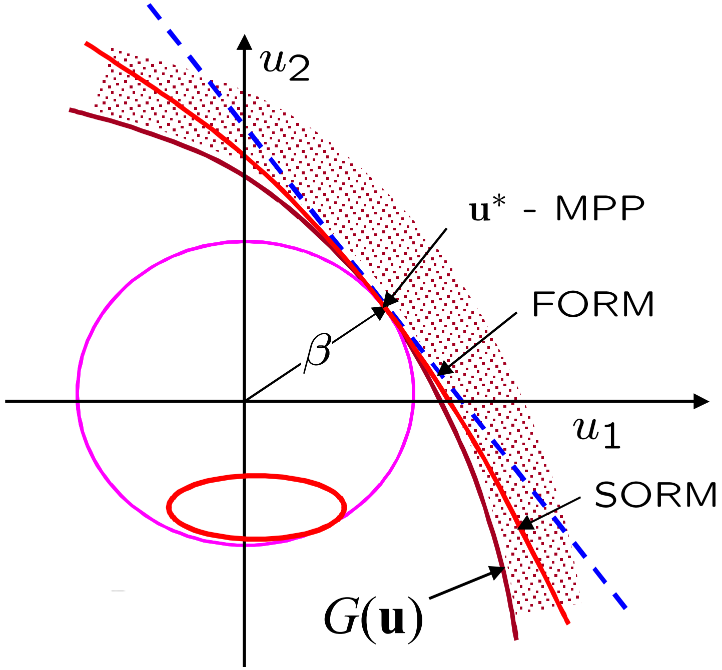
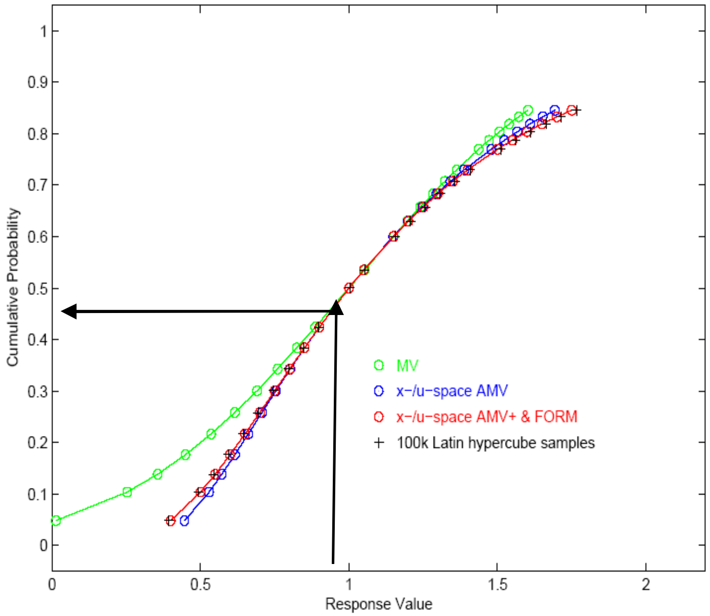
Analytic Reliability: MPP Search

Perform optimization **in u-space (std normal space corr. to uncertain x-space) to determine Most Probable Point (of response or failure occurring)**

Reliability Index
Approach (RIA)

$$\text{minimize} \quad \mathbf{u}^T\mathbf{u}$$
$$\text{subject to} \quad G(\mathbf{u}) = \bar{z}$$





...should yield better estimates of reliability than Mean Value methods

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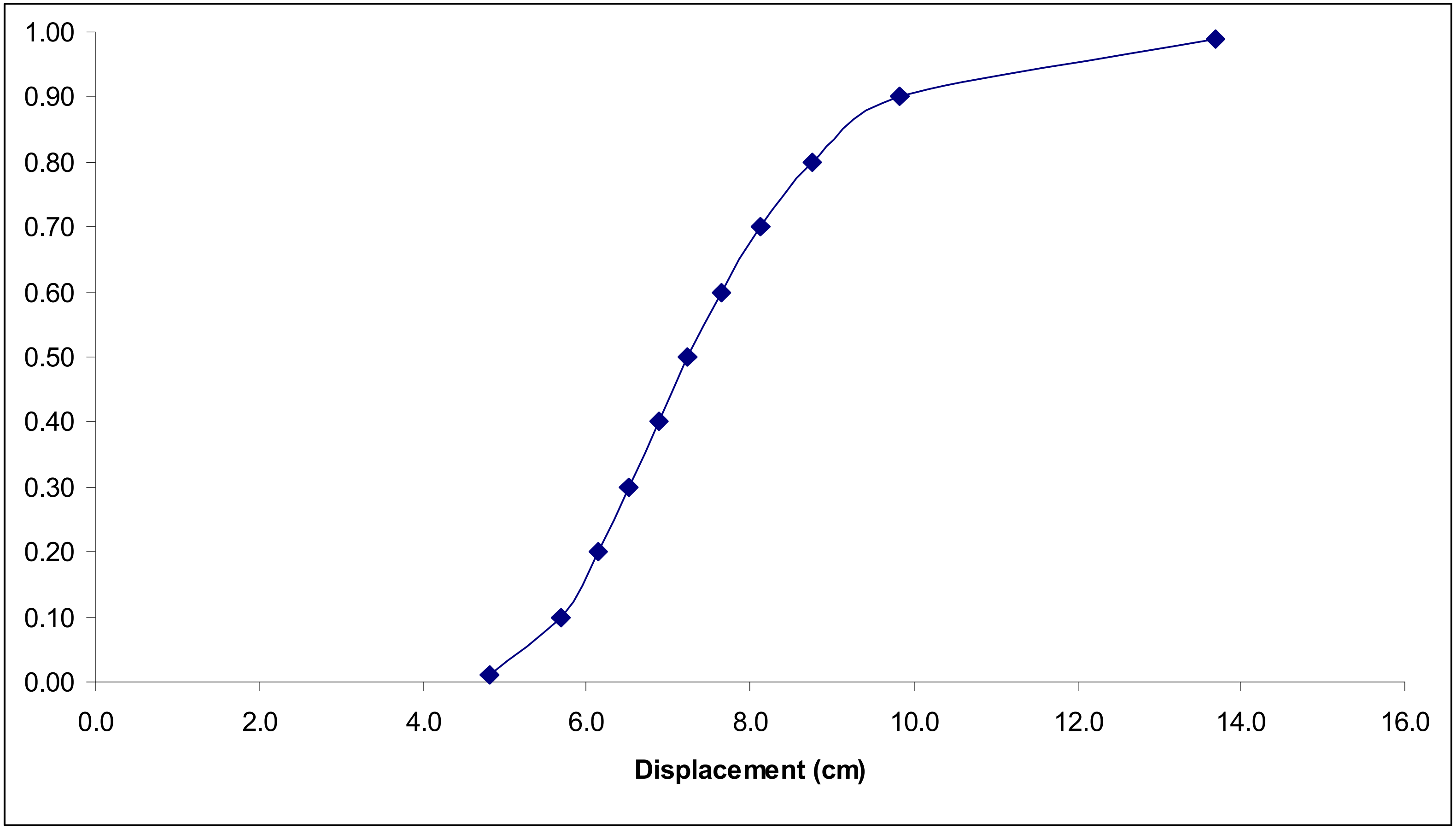
Analytic Reliability Results



Polynomial Chaos Expansions (PCE)

- **Represent a stochastic process (the uncertain output f(X)) as a spectral expansion in terms of suitable orthonormal eigenfunctions with weights associated with a particular density**

$$f(X) \approx \hat{a} = \sum_{k=0}^{P} a_k H_k^N(\xi)$$

- **The uncertain output f(X) is approximated by finite dimensional series based on unit Gaussian distributions**
- **In the expansion, the H terms are Hermite polynomials (multi-dimensional orthogonal polynomials), the ξ are standard normal random variables, and the coefficients a_k are deterministic but unknown.**
- **The job of PCE is to determine the coefficients a_k. Then, one has an approximation that can be sampled many times to calculate desired statistics**

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Polynomial Chaos Expansions (PCE)

Conceptually, the propagation of input uncertainty through a model using PCE in a non-intrusive approach consists of the following steps:

(1) Transform input uncertainties X to unit Gaussian random variables: X → ξ

(2) Assume a particular form for the orthogonal polynomials such as Hermite

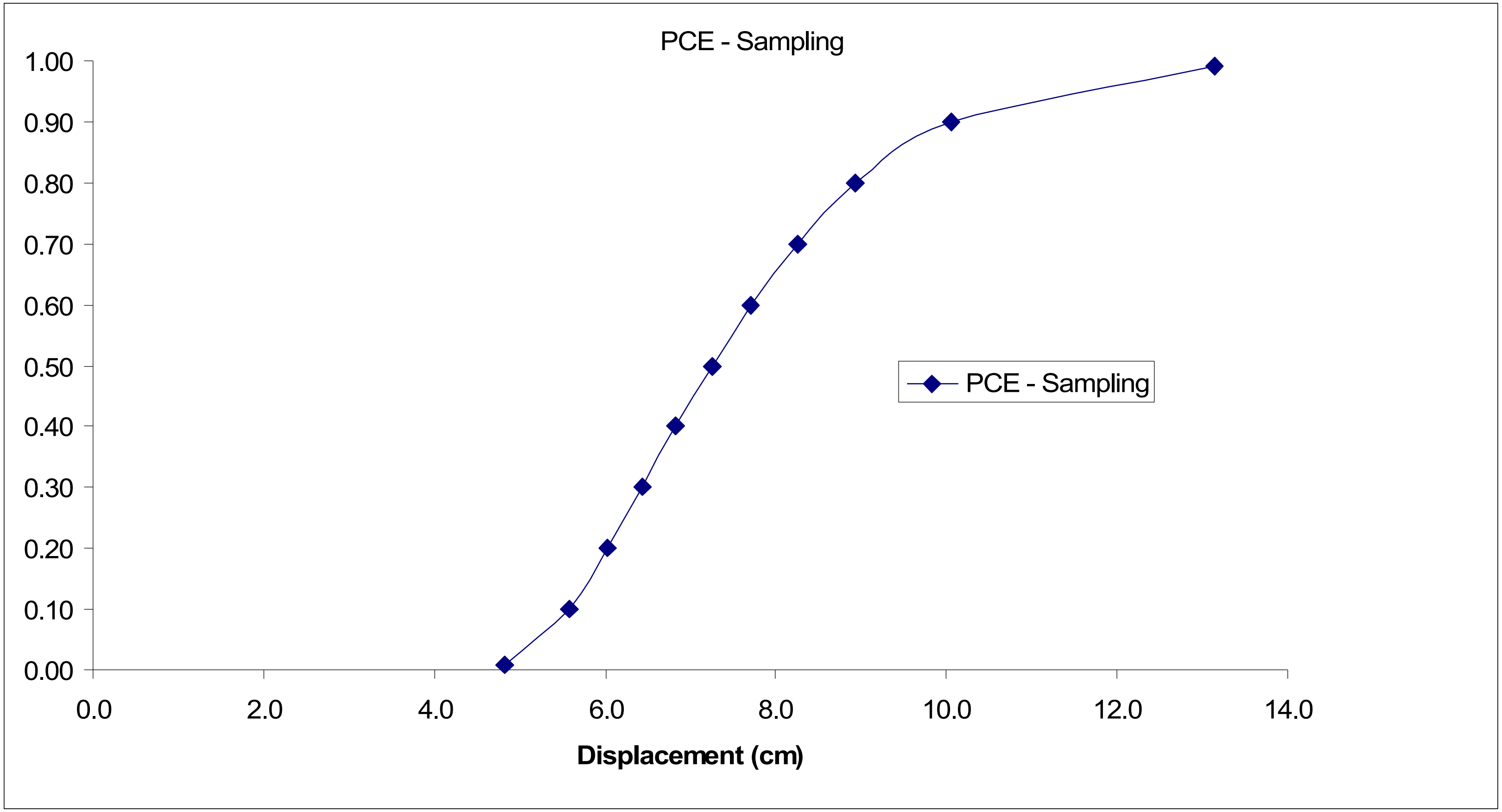
(3) Generate many samples of X and ξ. These will generate a a set of linear equations to solve for the spectral expansion coefficients

$$f(X_i) \approx \hat{a} = \sum_{k=0}^{P} a_k H_k^N(\xi_i) \quad \text{for i = 1…N samples}$$

(4) Once the coefficients ak are determined, take 1000s of samples of ξ and run them through the spectal expansion equation to obtain an approximation for f(X) → build up a CDF of f(X)

NOTE: In step 3, DAKOTA can build the PCE approximation based on LHS samples, quadrature points, collocation points, or on a set of points that the user has determined. These methods have pros and cons in terms of the efficiency and applicability. This is an active research area which we are still investigating.

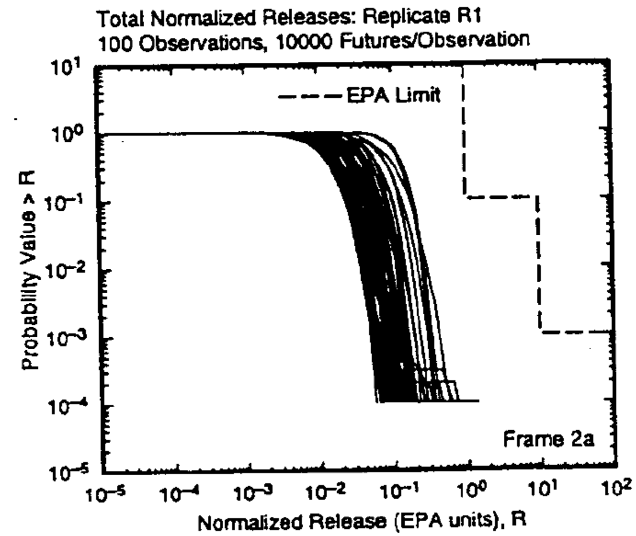
Polynomial Chaos Results



Epistemic UQ

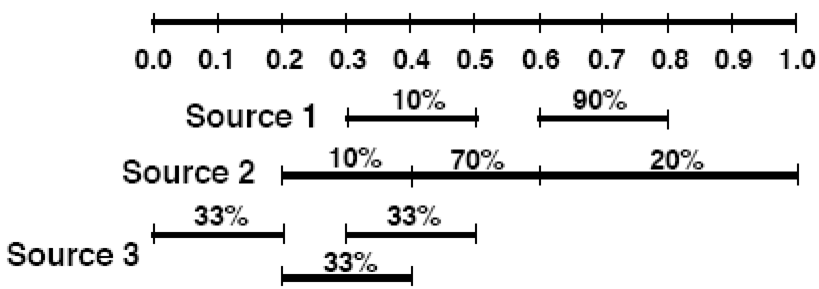
Second-order probability

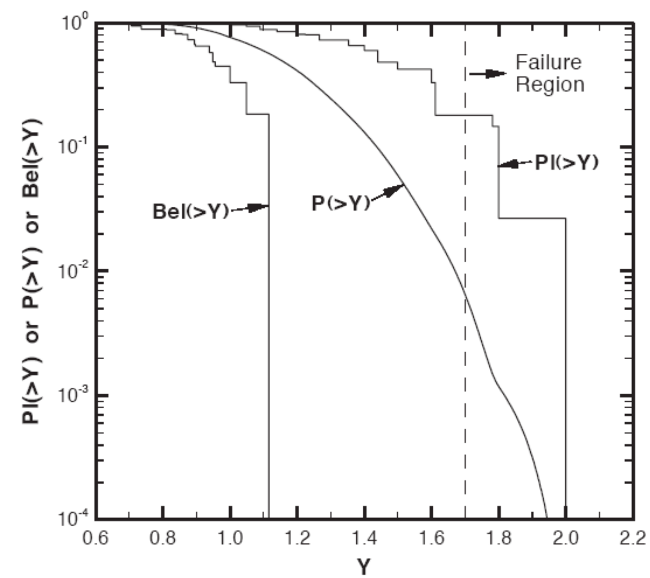
- Two levels: distributions/intervals on distribution parameters
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).



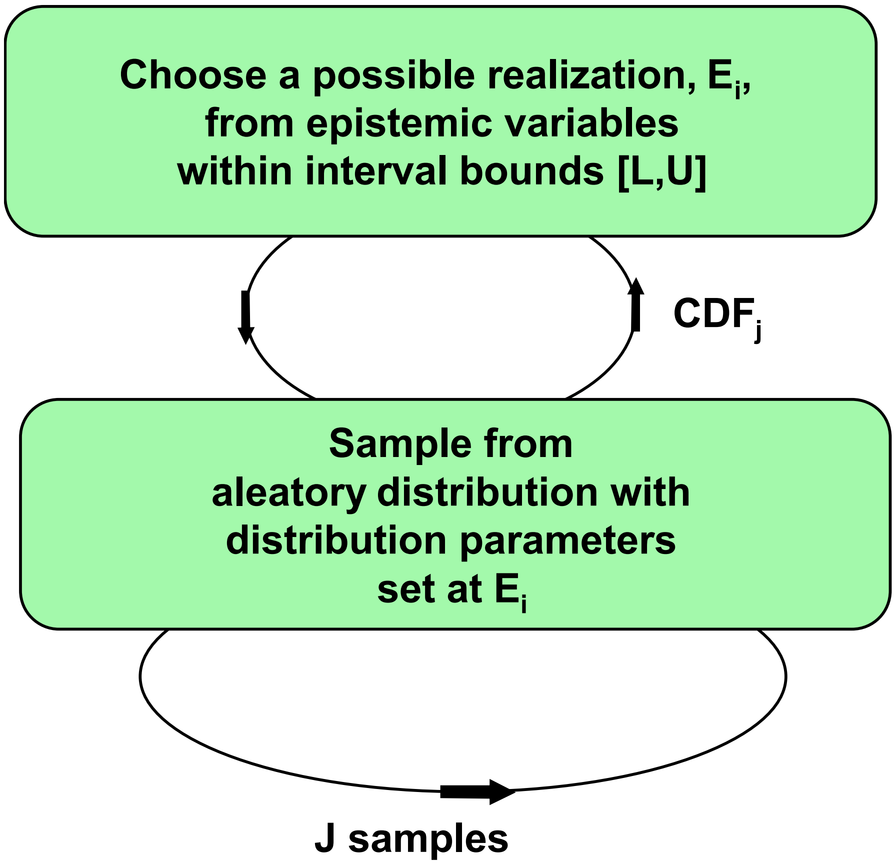
Dempster-Shafer theory of evidence

- Basic probability assignment (interval-based)
- Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals

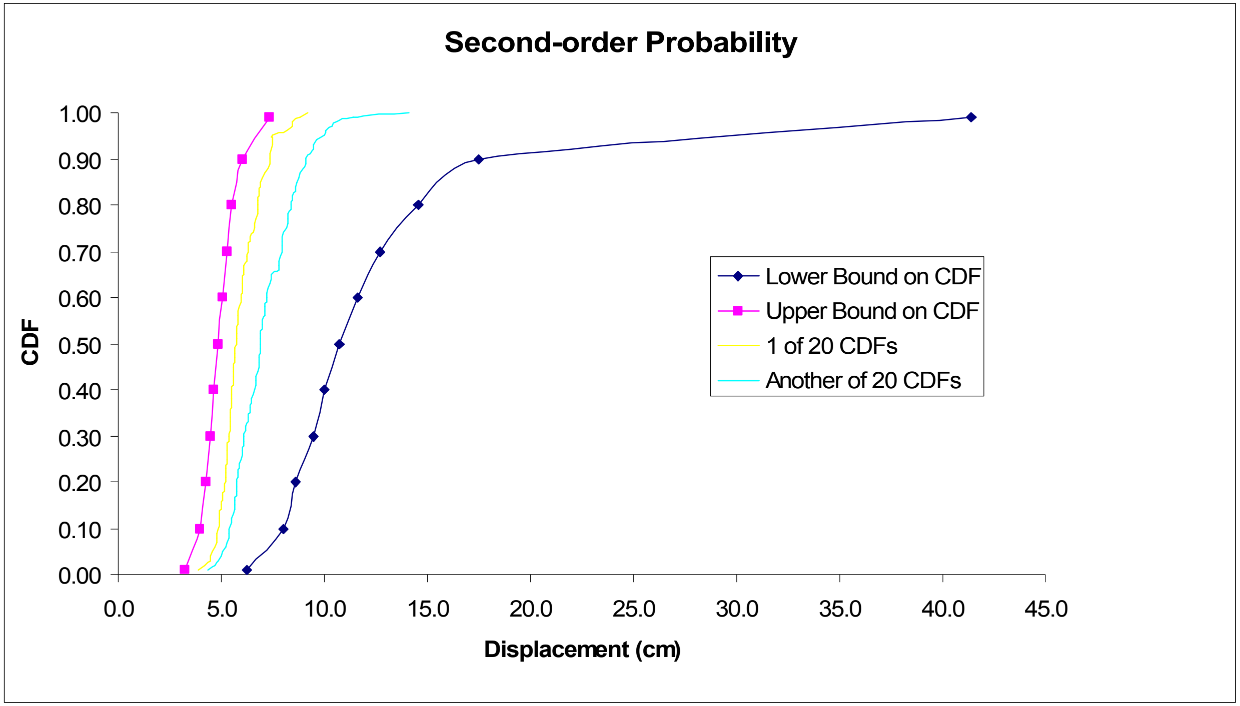




Second-order Probability



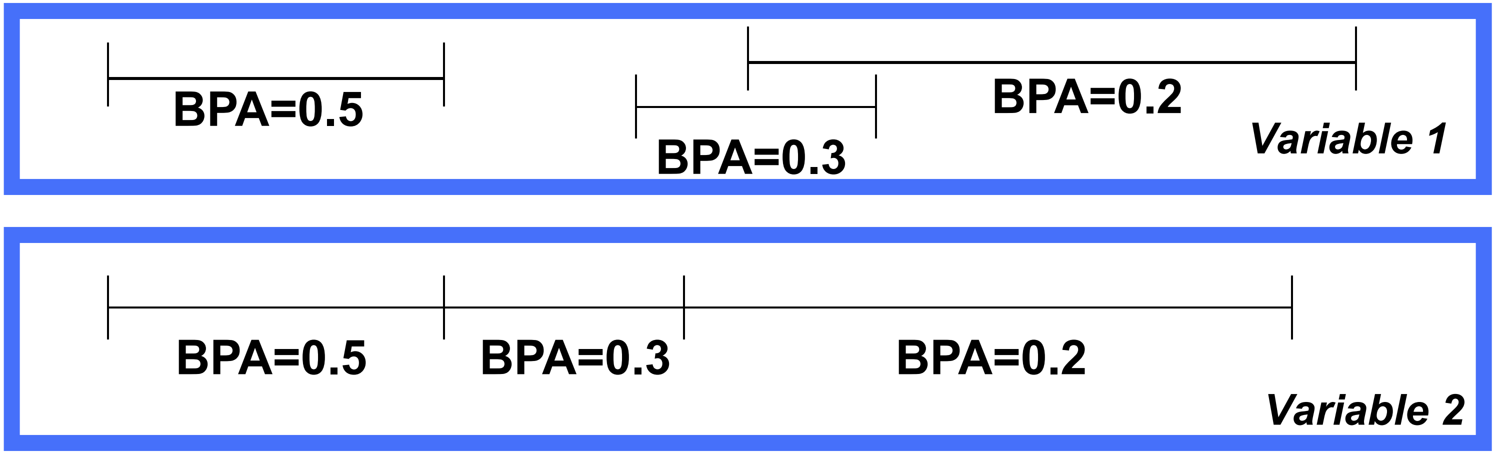
Second-order Probability



Variable	Epistemic Mean	Distribution
L	[0.98, 1.02] m	Normal(epistemic mean, 0.01) m
P	[90,110] N	Normal(epistemic mean, 5) N
E	[41.4,96,6] GPa	Normal(epistemic mean, 13.8) GPa

Epistemic Uncertainty Quantification

- Epistemic uncertainty refers to the situation where one does not know enough to specify a probability distribution on a variable
- Sometimes it is referred to as subjective, reducible, or lack of knowledge uncertainty
- Initial implementation in DAKOTA uses Dempster-Shafer belief structures. For each uncertain input variable, one specifies "basic probability assignment" for each potential interval where this variable may exist.
- Intervals may be contiguous, overlapping, or have "gaps"



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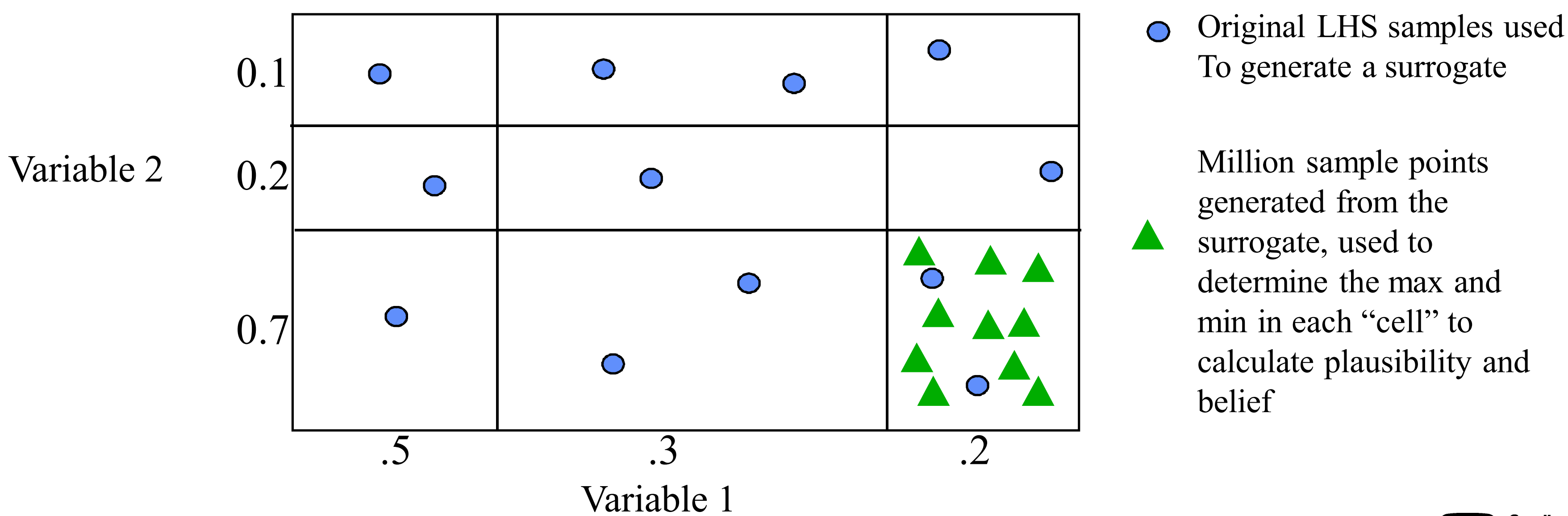
Epistemic Uncertainty Quantification

- Look at various combinations of intervals. In each joint interval “box”, one needs to find the maximum and minimum value in that box (by sampling or optimization)
- Belief is a lower bound on the probability that is consistent with the evidence
- Plausibility is the upper bound on the probability that is consistent with the evidence
- Order these beliefs and plausibility to get CDFs



Dempster-Shafer Example

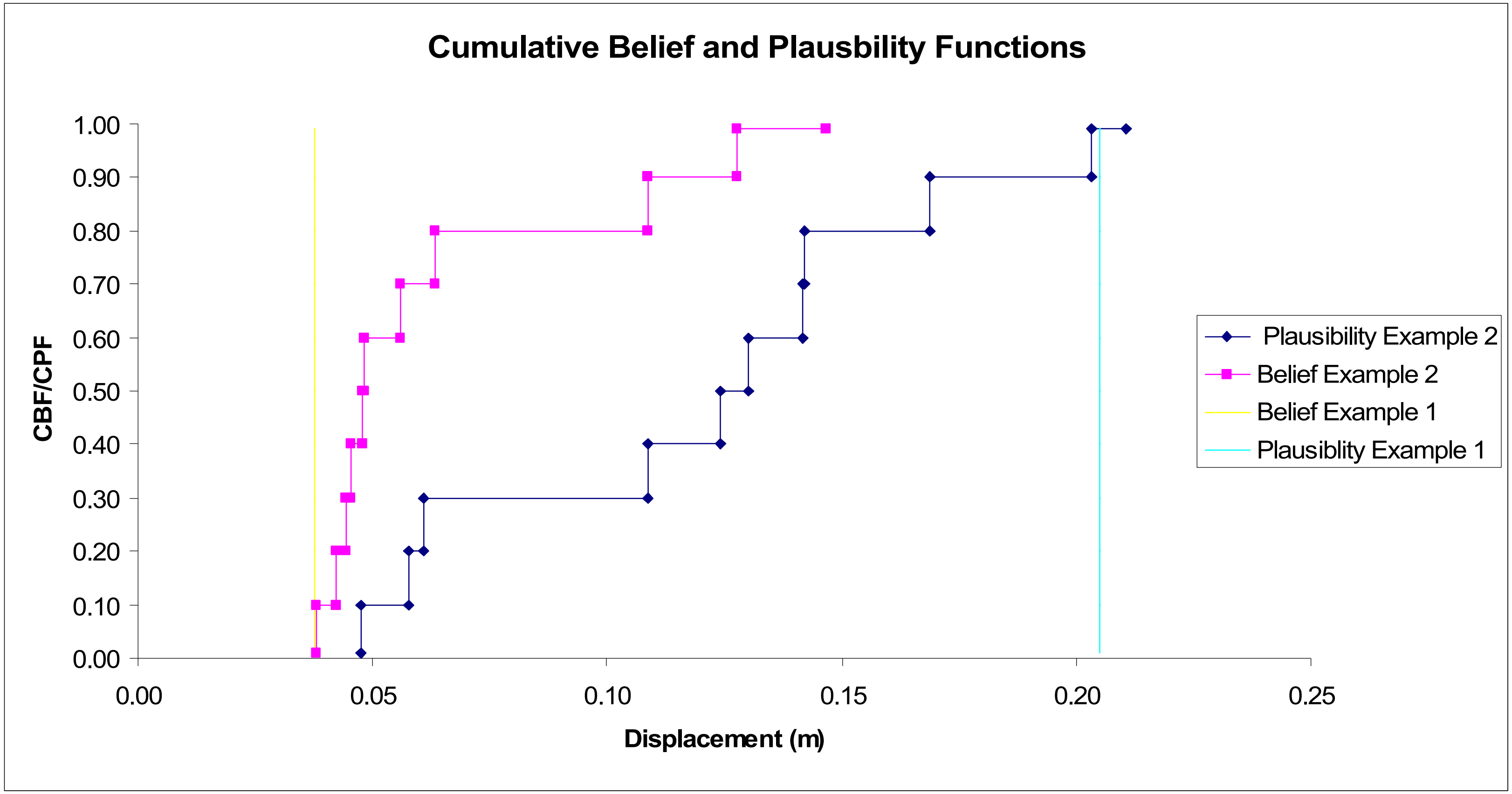
Variable	Intervals	BPA
L	[0.97, 1.03] m	1.0
P	[85,115] N	1.0
E	[27.6,110.4]GPa	1.0

Table 3a. Epistemic Variables for the Cantilever Beam Problem, Example 1

Variable	Intervals	BPA
L	[0.97, 0.98] [0.98, 1.02] [1.02,1.03] m	0.25, 0.5, 0.25
P	[85,90] [90,110] [110,115] N	0.25, 0.5, 0.25
E	[27.6,41.4] [41.4, 96.6] [96.6,110.4]GPa	0.25, 0.5, 0.25

Table 3b. Epistemic Variables for the Cantilever Beam Problem, Example 2

D-S Epistemic Uncertainty Results



Method Comparison

UQ Method Characteristics	Sampling	Analytic Reliability	Polynomial Chaos	Dempster-Shafer	Second- order Probability
Inputs specified by probability distribution	YES Wide range of distributions	YES Can handle many common distributions	YES, Only Gaussian distributions for many cases	NO	No for outer loop; yes for inner
Correlations amongst inputs	YES	In some cases	YES	NO	No for outer loop; yes for inner
Number of samples required for M uncertain inputs	(10-20) * M Note: the number of samples depends on the statistics of the output distribution being resolved. For accurate mean estimates, 30 -50 samples may be sufficient, whereas thousands of samples are needed to estimate a 99th percentile	No samples needed; number of function evaluations depends on the problem formulation and type of optimization used	(10-20)*M to be able to solve for coefficients	100K- 1Mill. Often ~100-1000 LHS samples are taken to construct a surrogate, and the surrogate is sampled millions of times	50-100 in outer loop * (10-20)*M in inner loop
Outputs	Output distribution (CDF) with moments	Probability of failure for a given response level	Functional form of output: Y=PCE(X). From this, one can calculate statistics of interest	Cumulative distribution function for plausibility and belief	Ensembles of CDFs; lower and upper bounds on possible CDF given epistemic uncertainty

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Summary

- UQ is more than sampling
- Sampling is at the basis of the more advanced methods
- Engineering analysts are starting to use more efficient aleatory methods and explore epistemic methods
- There is much confusion over the proper use and applicability of each method
- Example applications and case studies can be used to help deploy UQ methods

DAKOTA Team Contact Info

- Web site:
  - http://endo.sandia.gov/DAKOTA
  - Email: dakota@sandia.gov
  - User's Manual, Reference Manual, Developers Manual - online

- Team Members
  - Mike Eldred, Principal Investigator (R&D)
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  - Shane Brown, Support Manager (software issues)
  - Laura Swiler
  - Brian Adams
  - Danny Dunlavy
  - Dave Gay
  - Bill Hart
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  - Many other technical contributors (SNL-CA, SNL-NM, academia,...)
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  - Marty Pilch, Dept. 1533 manager