SAND 2009-0511P

DAKOTA Training

Uncertainty Quantification (UQ)

http://www.cs.sandia.gov/dakota

Learning outcomes:

- **Understand terminology, goals, and applications of UQ methods**
- **Use DAKOTA's workhorse sampling method (LHS) to compute statistics and probability distributions with the Rosenbrock function**
- **Differentiate reliability methods and stochastic expansion methods; run studies demonstrating benefit over LHS**
- **Epistemic uncertainty: understand DAKOTA approaches for lack-of-knowledge uncertainty**

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Risk-informed Decision Making, QMU, and UQ

The following are essential to support risk-informed decision making using modeling and simulation:

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

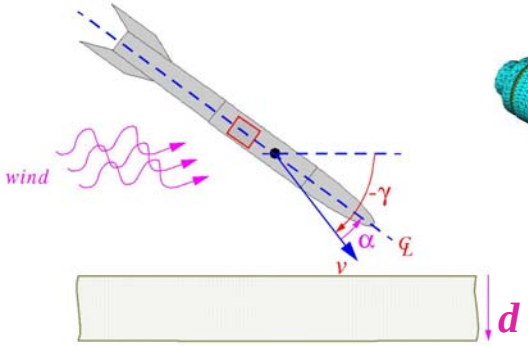
Formal DOE process for Quantification of Margins and Uncertainties (QMU): process of quantifying the impact of uncertainties in the decision context

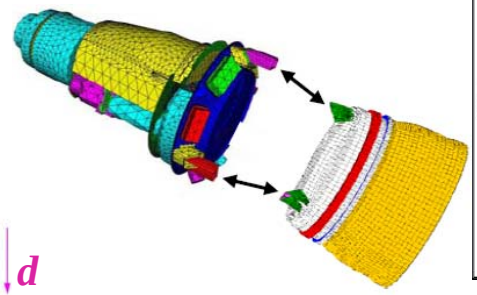
Uncertainty Quantification

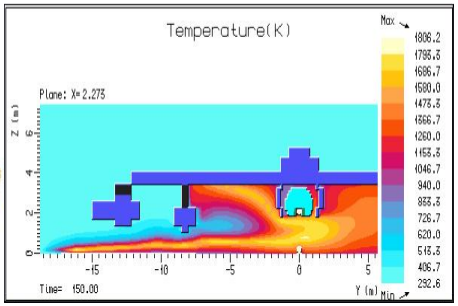
Critical component of QMU: credible M&S capability for stockpile stewardship

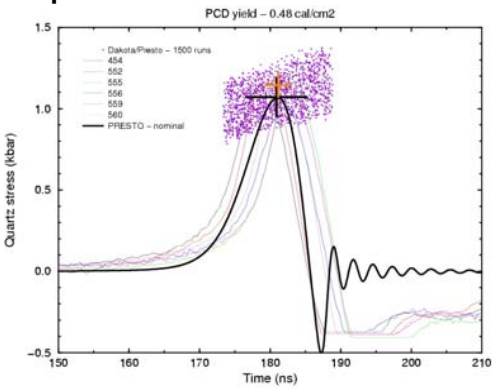
Two categories of uncertainty:

- **Aleatory/irreducible:** inherent variability with sufficient data → probabilistic models
- **Epistemic/reducible:** uncertainty from lack of knowledge → nonprobabilistic models





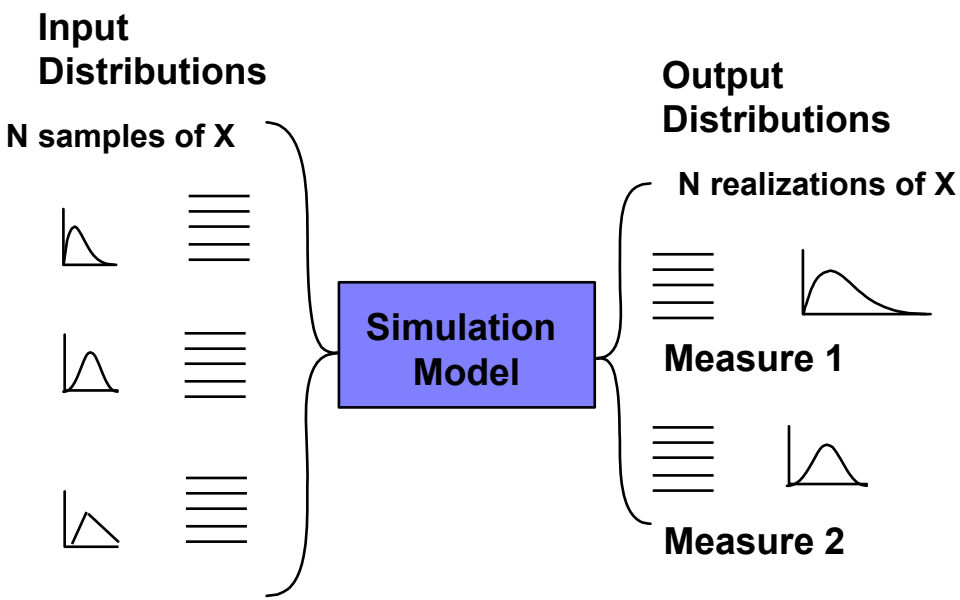


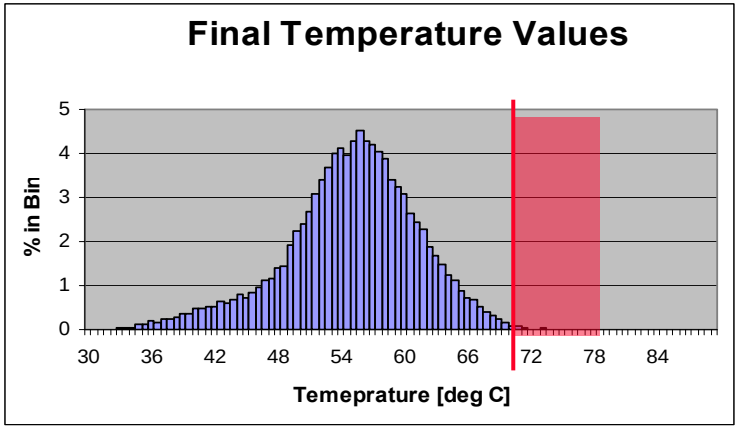


Uncertainty applications: penetration, joint mechanics, abnormal environments, shock physics, …

Sampling

- **Assume distributions on the uncertain input values, repeatedly sample from those distributions and run the model with the sampled values;** ***yields corresponding distributions of the outputs***
- **Considerable work has led to more efficient Monte Carlo sampling methods, including stratified sampling (Latin hypercube sampling) or quasi-Monte Carlo sampling which spread the samples over the space.**
- **Sampling is not the most efficient UQ method, but is easy to implement and transparent in terms of tracing sample realizations through multiple codes for complex UQ studies.**



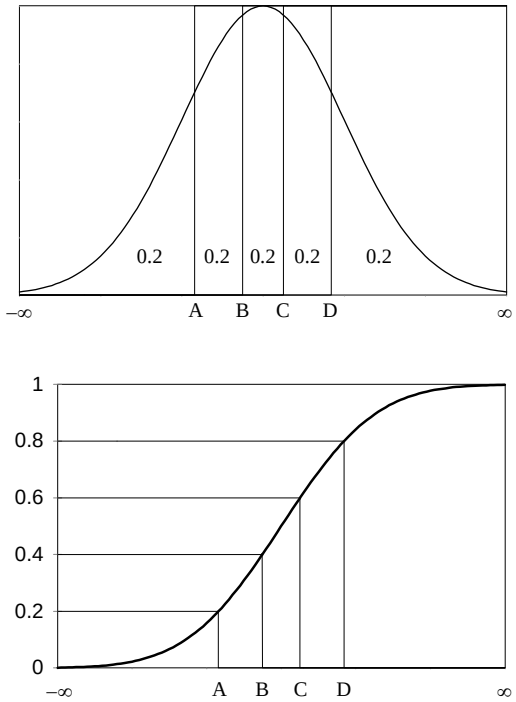


Goals: assess nominal, variability, tail statistics, probability of failure

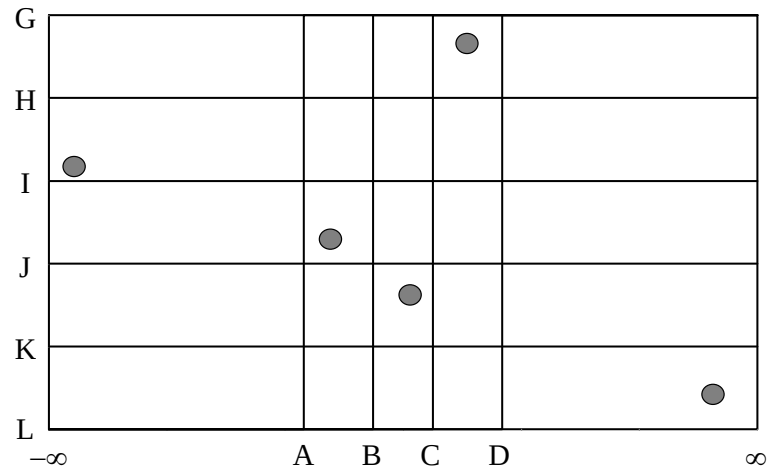
Sandia National Laboratories

Latin Hypercube Sampling

- Early work by McKay and Conover
- Restricted pairing by Iman
- Monte Carlo (MC) sampling
- LHS is stratified random sampling among equal probability bins for all 1-D projections of an n-dimensional set of samples.



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



A Two-Dimensional Representation of One Possible LHS of size 5 Utilizing X1 (normal) and X2 (uniform)

Example Input/Output: Sampling

```
strategy,
    single_method
      graphics
      tabular_graphics_data

method,
    nond_sampling
    samples = 200 seed = 17
    sample_type random
    response_levels = 100.0

model,
    single

variables,
    uniform_uncertain = 2
     lower_bounds -2.0  -2.0
     upper_bounds  2.0   2.0
     descriptor s       'x1'  'x2'

interface,
    direct
      analysis_driver = 'rosenbrock‘

responses,
    num_response_functions = 1
    no_gradients
    no_hessians
```

Sampling Input (examples/tutorial/dakota_rosenbrock_nond.in)

```
Statistics based on 200 samples:

Moments for each response function:
response_fn_1:  Mean = 4.43855e+02  Std. Dev. = 5.88920e+02  Coeff. of
Variation = 1.32683e+00

95% confidence intervals for each response function:
response_fn_1:  Mean = ( 3.61736e+02, 5.25973e+02 ), Std Dev = ( 5.36308e+02,
6.53068e+02 )

Probabilities for each response function:
Cumulative Distribution Function (CDF) for response_fn_1:
     Response Level      Probability Level  Reliability Index  General Rel Index
     --------------      -----------------  -----------------  -----------------
   1.0000000000e+02   3.7000000000e-01

Simple Correlation Matrix among all inputs and outputs:
                    x1          x2 response_fn_1
          x1  1.00000e+00
          x2 -4.33667e-03  1.00000e+00
response_fn_1  6.45646e-02 -4.81363e-01  1.00000e+00

Partial Correlation Matrix between input and output:
             response_fn_1
          x1  7.12791e-02
          x2 -4.82094e-01
```

Sampling Output

Exercise: DAKOTA Monte Carlo

- Examine the input file
  `examples/tutorial/dakota_rosenbrock_nond.in`
- Run the problem:
  `>> dakota –i dakota_rosenbrock_nond.in –o this.out`
- Look at output files `this.out` and `dakota_tabular.dat`

- Now edit the input file
  - change `sampling_type random` to `sampling_type lhs`
  - change `uniform_uncertain` to `normal_uncertain`, and `lower_bounds` to `means = 0. 0.`, `upper_bounds` to `std_deviations = 1.0 1.0`

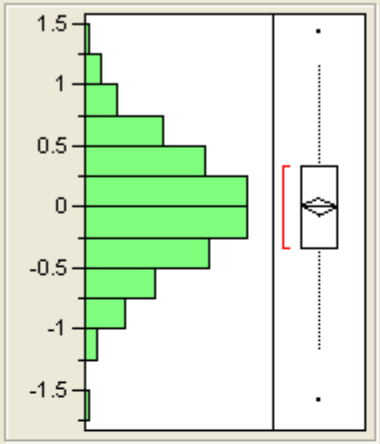
- Can change the seed and the number of samples to see how the outputs (mean, std deviation, correlations) change as well

User's Manual Section 2.4.9

Example Postprocessing of Samples

Distributions

X1



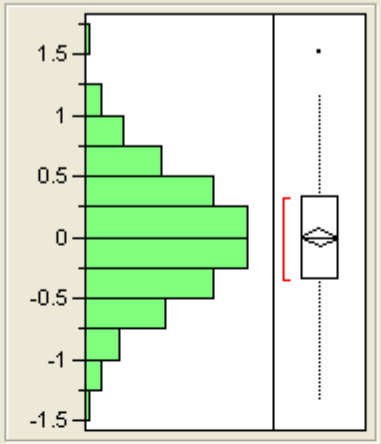
Quantiles

100.0%	maximum	1.432
99.5%		1.431
97.5%		1.004
90.0%		0.653
75.0%	quartile	0.336
50.0%	median	0.00111
25.0%	quartile	-0.338
10.0%		-0.643
2.5%		-0.981
0.5%		-1.583
0.0%	minimum	-1.585

Moments

Mean	-0.000554
Std Dev	0.5013361
Std Err Mean	0.0354498
upper 95% Mean	0.0693512
lower 95% Mean	-0.07046
N	200

X2



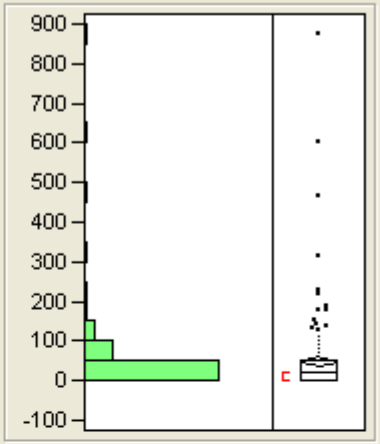
Quantiles

100.0%	maximum	1.512
99.5%		1.511
97.5%		1.009
90.0%		0.648
75.0%	quartile	0.339
50.0%	median	-0.0009
25.0%	quartile	-0.340
10.0%		-0.641
2.5%		-1.017
0.5%		-1.318
0.0%	minimum	-1.319

Moments

Mean	0.000567
Std Dev	0.499207
Std Err Mean	0.0352993
upper 95% Mean	0.0701756
lower 95% Mean	-0.069042
N	200

Rosenbrock



Quantiles

100.0%	maximum	872.82
99.5%		871.48
97.5%		229.36
90.0%		104.96
75.0%	quartile	52.65
50.0%	median	20.62
25.0%	quartile	3.45
10.0%		1.90
2.5%		0.78
0.5%		0.51
0.0%	minimum	0.51

Moments

Mean	46.827002
Std Dev	91.39245
Std Err Mean	6.4624221
upper 95% Mean	59.570617
lower 95% Mean	34.083386
N	200

Latin Hypercube Sampling

- LHS allows the following distributions in DAKOTA:
  - Uniform
  - Loguniform
  - Normal (bounded)
  - Lognormal (bounded)
  - Triangular
  - Exponential
  - Beta
  - Gamma
  - Weibull
  - Frechet – Extreme value
  - Gumbel – Extreme value
  - Histogram – bin values or point pairs
  - Interval – use only in epistemic analysis
- There is a standalone LHS driver in Dakota/bin/lhsdrv
- Use this if you only want to generate samples

Recipe for a DAKOTA Sampling Study

- **Define parameter ranges and/or probability distributions.**

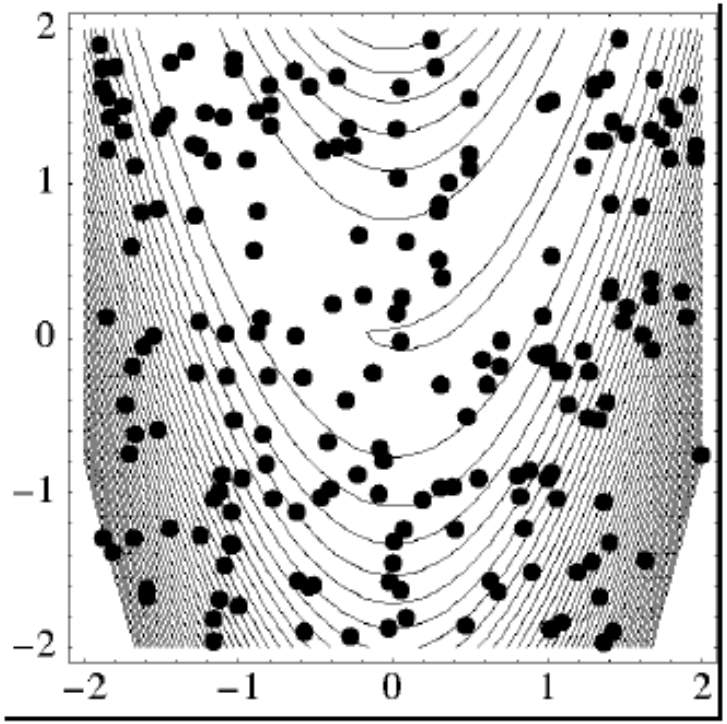
- **Use the Latin hypercube sampling method to generate Order(N to N^2) samples of the x-values.**
  - **For a good estimate of mean response, 30-50 samples will likely suffice**
  - **For a good estimate of variance, 200-300 samples will likely suffice**
  - **One rule of thumb is: ~10—30 samples for each N (# samples = 10*N or 30*N)**
  - **Another is: # samples = 1/3 of simulation run budget, saving the other 2/3 for follow-on studies**

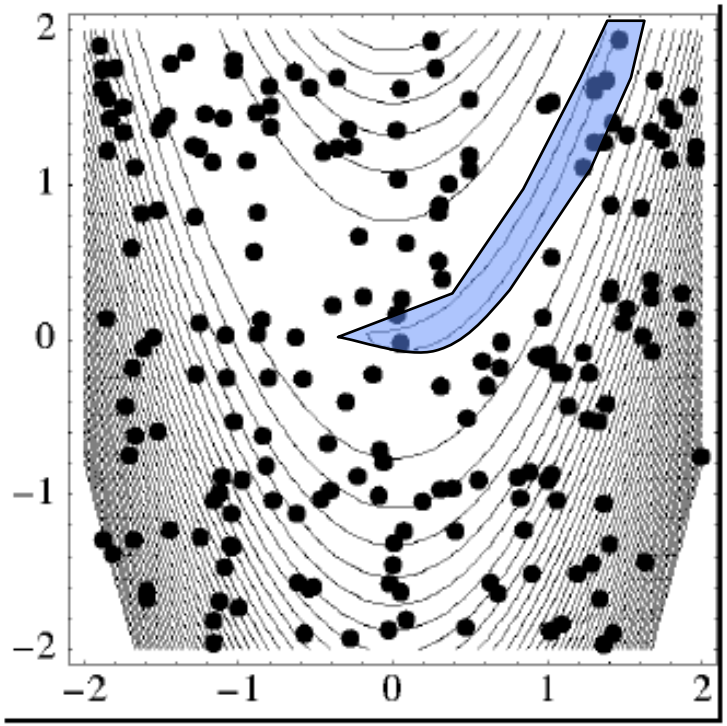
- **Examine the f-value correlation data and basic statistical data generated by DAKOTA.**
  - **These correlations are the "global" linear trends in the f-values.**
  - **Often they are useful in finding a worst-case or best-case combination of x-values.**

- **Perform a more detailed statistical analysis**

- ***Only use DAKOTA's f-value probability estimates if you have well-founded knowledge about the probability distributions on the x-values.***

Sampling for Sensitivity Analysis vs. UQ





We only know the bounds, and not any probabilities on x1 and x2.

- **Get correlations, min, max, and trend data**

We assume some probability distributions on x1 and x2.

- **Get correlations, min, max, and trend data**
- **Also can analyze the probability distribution of the output: DAKOTA produces statistics on the f-values (e.g., Prob(f<4) = 0.049)**

Sandia National Laboratories

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

	Production	New	Under dev.	Planned	Collabs.
Sampling	LHS/MC, QMC/CVT	IS/AIS/MMAIS, Incremental LHS		Bootstrap, Jackknife	Gunzburger
Reliability	*1st/2nd-order local:* MV/MV^2, x/u AMV/AMV^2/AMV+/ AMV^2+, x/u TANA, FORM/SORM	*Global:* EGRA			*Local:* Renaud, *Global:* Mahadevan
Stochastic expansion		*gPCE:* sampling, pt colloc, quad, sparse grid. *SC:* quad, sparse grid	*gPCE:* tailored exp. gPCE/SC: anisotropic sparse grid	*gPCE/SC:* arbitrary input PDFs, adaptivity	Ghanem, Burkardt, Iaccarino, Maute, Xiu
Other probabilistic		Random fields/ stochastic proc.		Dimension reduction	Grigoriu, Youn
Epistemic	Second-order probability	Dempster-Shafer evidence theory	Opt-based interval est.	Bayesian, Imprecise probability	Higdon, Williams, Ferson
Metrics	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		Storlie

UQ with Reliability Methods

Mean Value Method

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

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

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

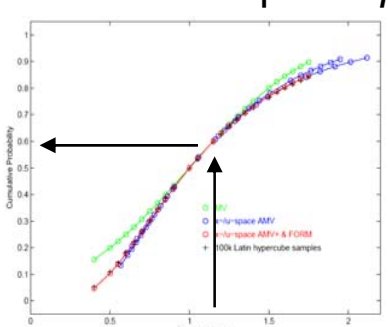
Rough statistics

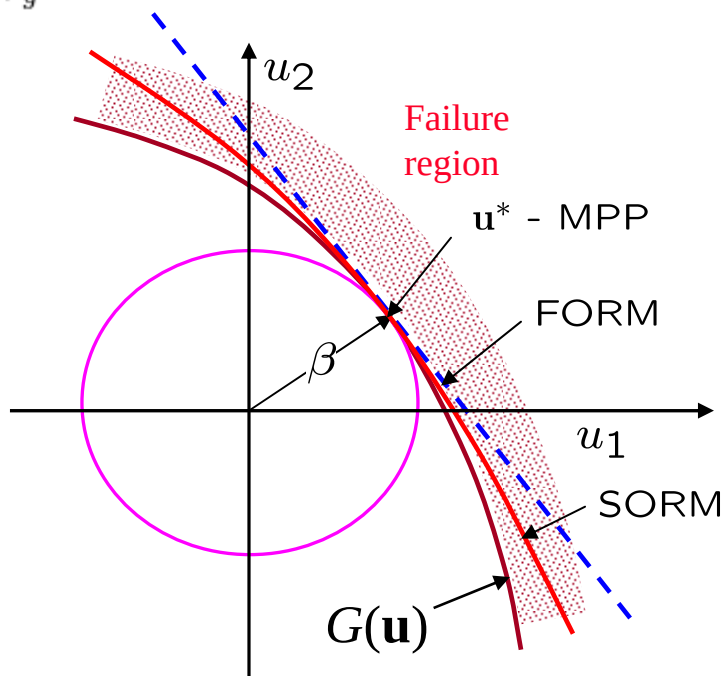
MPP search methods

Reliability Index Approach (RIA)

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

Find min dist to *G* level curve
Used for fwd map *z* → *p*/*β*



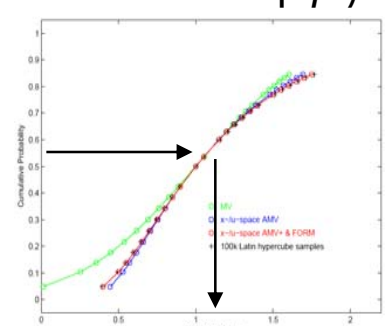


Nataf x → u: $\Phi(z_i) = F(x_i)$
$\mathbf{z} = \mathbf{L}\mathbf{u}$

Performance Measure Approach (PMA)

$$\text{minimize} \quad \pm G(\mathbf{u})$$
$$\text{subject to} \quad \mathbf{u}^T \mathbf{u} = \bar{\beta}^2$$

Find min *G* at *β* radius
Used for inv map *p*/*β* → *z*



Sandia National Laboratories

Reliability Algorithm Variations: First-Order Methods

Limit state linearizations

AMV: $g(\mathbf{x}) = g(\mu_\mathbf{x}) + \nabla_x g(\mu_\mathbf{x})^T(\mathbf{x} - \mu_\mathbf{x})$

u-space AMV: $G(\mathbf{u}) = G(\mu_\mathbf{u}) + \nabla_u G(\mu_\mathbf{u})^T(\mathbf{u} - \mu_\mathbf{u})$

AMV+: $g(\mathbf{x}) = g(\mathbf{x}^*) + \nabla_x g(\mathbf{x}^*)^T(\mathbf{x} - \mathbf{x}^*)$

u-space AMV+: $G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T(\mathbf{u} - \mathbf{u}^*)$

FORM: no linearization

Integrations

1st-order: $\begin{cases} p(g \leq z) & = & \Phi(-\beta_{cdf}) \\ p(g > z) & = & \Phi(-\beta_{ccdf}) \end{cases}$

MPP search algorithm

[HL-RF], Sequential Quadratic Prog. (SQP), Nonlinear Interior Point (NIP)

Warm starting

When: **AMV+ iteration increment, *z/p/β* level increment, or design variable change**

What: **linearization point & assoc. responses (AMV+) and MPP search initial guess**

MPP initial guess benefits from *projection* since KKT conditions w.r.t. **u** still satisfied for new level at previous optimum

RIA Projection:

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \alpha \nabla_u G(\mathbf{u}^{(k)})$$

$$\alpha = \frac{G^{(k+1)} - G^{(k)}}{\|\nabla_u G(\mathbf{u}^{(k)})\|^2}$$

PMA Projection:

$$\mathbf{u}^{(k+1)} = \frac{\beta^{(k+1)}}{\beta^{(k)}}\mathbf{u}^{(k)}$$

Eldred, M.S., Agarwal, H., Perez, V.M., Wojtkiewicz, S.F., Jr., and Renaud, J.E., Investigation of Reliability Method Formulations in DAKOTA/UQ, (to appear) *Structure and Infrastructure Engineering*, Taylor & Francis.

Reliability Algorithm Variations: Second-Order Methods

2nd-order local limit state approximations

- e.g., x-space AMV²+:

$$g(\mathrm{x}) \cong g(\mathrm{x}^*) + \nabla_x g(\mathrm{x}^*)^T(\mathrm{x}-\mathrm{x}^*) + \frac{1}{2}(\mathrm{x}-\mathrm{x}^*)^T \nabla_x^2 g(\mathrm{x}^*)(\mathrm{x}-\mathrm{x}^*)$$

- Hessians may be full/FD/Quasi
- Quasi-Newton Hessians may be BFGS or SR1

Multipoint limit state approximations

- e.g., TPEA, TANA:

$$g(\mathrm{x}) \cong g(\mathrm{x}_2) + \sum_{i=1}^{n} \frac{\partial g}{\partial x_i}(\mathrm{x}_2) \frac{x_{i,2}^{1-p_i}}{p_i}(x_i^{p_i} - x_{i,2}^{p_i}) + \frac{1}{2}\epsilon(\mathrm{x}) \sum_{i=1}^{n}(x_i^{p_i} - x_{i,2}^{p_i})^2$$

$$p_i = 1 + \ln\left[\frac{\frac{\partial g}{\partial x_i}(\mathrm{x}_1)}{\frac{\partial g}{\partial x_i}(\mathrm{x}_2)}\right] \Big/ \ln\left[\frac{x_{i,1}}{x_{i,2}}\right]$$

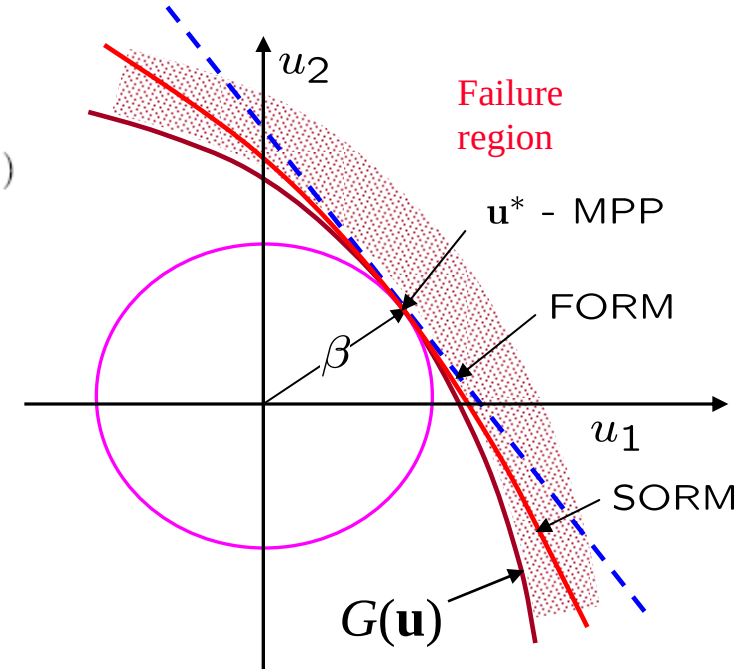
$$\epsilon(\mathrm{x}) = \frac{H}{\sum_{i=1}^{n}(x_i^{p_i} - x_{i,1}^{p_i})^2 + \sum_{i=1}^{n}(x_i^{p_i} - x_{i,2}^{p_i})^2}$$

$$H = 2\left[g(\mathrm{x}_1) - g(\mathrm{x}_2) - \sum_{i=1}^{n} \frac{\partial g}{\partial x_i}(\mathrm{x}_2) \frac{x_{i,2}^{1-p_i}}{p_i}(x_{i,1}^{p_i} - x_{i,2}^{p_i})\right]$$

2nd-order integrations

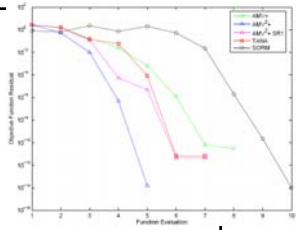
$$p = \Phi(-\beta) \underbrace{\prod_{i=1}^{n-1} \frac{1}{\sqrt{1+\beta\kappa_i}}}_{\text{curvature correction}}$$

Also, AIS, …



Synergistic features:

Hessian data needed for SORM integration can enable more rapid MPP convergence



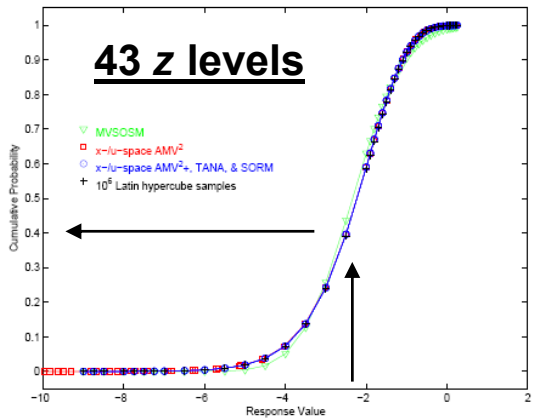
[QN] Hessian data accumulated during MPP search can enable more accurate probability estimates

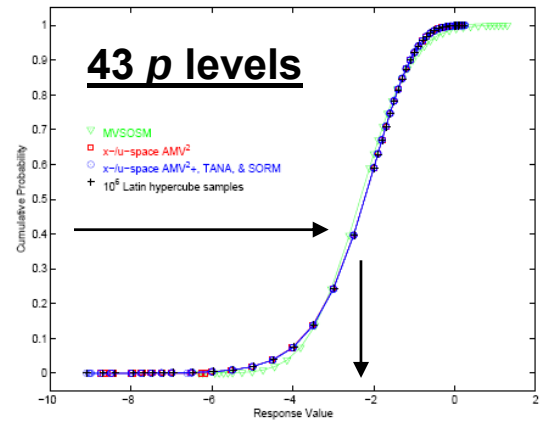
Eldred, M.S. and Bichon, B.J., Second-Order Reliability Formulations in DAKOTA/UQ, (in review)
Structure and Infrastructure Engineering, special issue on uncertainty in aerospace systems, Taylor & Francis.

Sandia National Laboratories

Reliability Algorithm Variations: Sample Results

Analytic benchmark test problems: lognormal ratio, short column, cantilever





RIA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF p Error Norm	Target z Offset Norm
MVFOSM	1	1	0.1548	0.0
MVSOSM	1	1	0.1127	0.0
x-space AMV	45	45	0.009275	18.28
u-space AMV	45	45	0.006408	18.81
x-space AMV^2	45	45	0.002063	2.482
u-space AMV^2	45	45	0.001410	2.031
x-space AMV+	192	192	0.0	0.0
u-space AMV+	207	207	0.0	0.0
x-space AMV^2+	125	131	0.0	0.0
u-space AMV^2+	122	130	0.0	0.0
x-space TANA	245	246	0.0	0.0
u-space TANA	296*	278*	6.982e-5	0.08014
FORM	626	176	0.0	0.0
SORM	669	219	0.0	0.0

PMA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF z Error Norm	Target p Offset Norm
MVFOSM	1	1	7.454	0.0
MVSOSM	1	1	6.823	0.0
x-space AMV	45	45	0.9420	0.0
u-space AMV	45	45	0.5828	0.0
x-space AMV^2	45	45	2.730	0.0
u-space AMV^2	45	45	2.828	0.0
x-space AMV+	171	179	0.0	0.0
u-space AMV+	205	205	0.0	0.0
x-space AMV^2+	135	142	0.0	0.0
u-space AMV^2+	132	139	0.0	0.0
x-space TANA	293*	272	0.04259	1.598e-4
u-space TANA	325*	311*	2.208	5.600e-4
FORM	720	192	0.0	0.0
SORM	535	191*	2.410	6.522e-4

Note: 2nd-order PMA with prescribed p level is harder problem → requires $\beta(p)$ update/inversion

Local Reliability Example

- Compare sampling methods to local reliability methods (modify dakota_rosenbrock_nond.in or see examples/methods/dakota_uq_reliability.in)

Example Input/Output: Reliability

```
strategy,
        single_method graphics

method,
          nond_local_reliability
          mpp_search no_approx
           response_levels = .4 .5 .55 .6 .65 .7  .75 .8  .85
.9 1. 1.05 1.15 1.2 1.25 1.3 1.35 1.4 1.5 1.55 1.6 1.65
1.7 1.75

variables,
        lognormal_uncertain = 2
           means              =  1.  1
           std_deviations     =  0.5 0.5
           descriptors        =  'TF1ln'   'TF2ln'
           uncertain_correlation_matrix =      1   0.3
                                               0.3  1

interface,
                    system asynch
                      analysis_driver = 'log_ratio'

responses,
                    num_response_functions = 1
                    numerical_gradients
                      method_source dakota
                      interval_type central
                      fd_gradient_step_size = 1.e-4
```

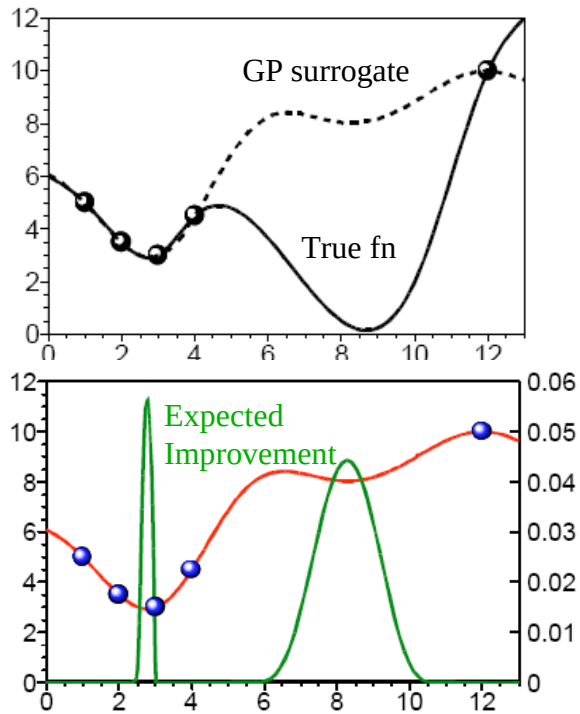
Reliability Input (examples/methods/dakota_uq_reliability.in)

```
<<<<< Iterator nond_local_reliability completed.
<<<<< Function evaluation summary: 657 total (561 new, 96 duplicate)
-----------------------------------------------------------------
Cumulative Distribution Function (CDF) for response_fn_1:
    Response Level  Probability Level  Reliability Index  General Rel Index
    --------------  -----------------  -----------------  -----------------
   4.0000000000e-01   4.7624085962e-02   1.6683404020e+00   1.6683404020e+00
   5.0000000000e-01   1.0346525475e-01   1.2620507942e+00   1.2620507942e+00
   5.5000000000e-01   1.3818404972e-01   1.0885143628e+00   1.0885143628e+00
   6.0000000000e-01   1.7616275822e-01   9.3008801339e-01   9.3008801339e-01
   6.5000000000e-01   2.1641741368e-01   7.8434989944e-01   7.8434989944e-01
   7.0000000000e-01   2.5803428381e-01   6.4941748143e-01   6.4941748143e-01
   7.5000000000e-01   3.0020938124e-01   5.2379840557e-01   5.2379840557e-01
   8.0000000000e-01   3.4226491013e-01   4.0628960782e-01   4.0628960782e-01
   8.5000000000e-01   3.8365052982e-01   2.9590705956e-01   2.9590705956e-01
   9.0000000000e-01   4.2393548232e-01   1.9183562480e-01   1.9183562480e-01
   1.0000000000e+00   5.0000000000e-01   4.7212046773e-12   4.7212177145e-12
   ...
```

Reliability Output

New UQ Method:
Efficient Global Reliability Analysis (EGRA)

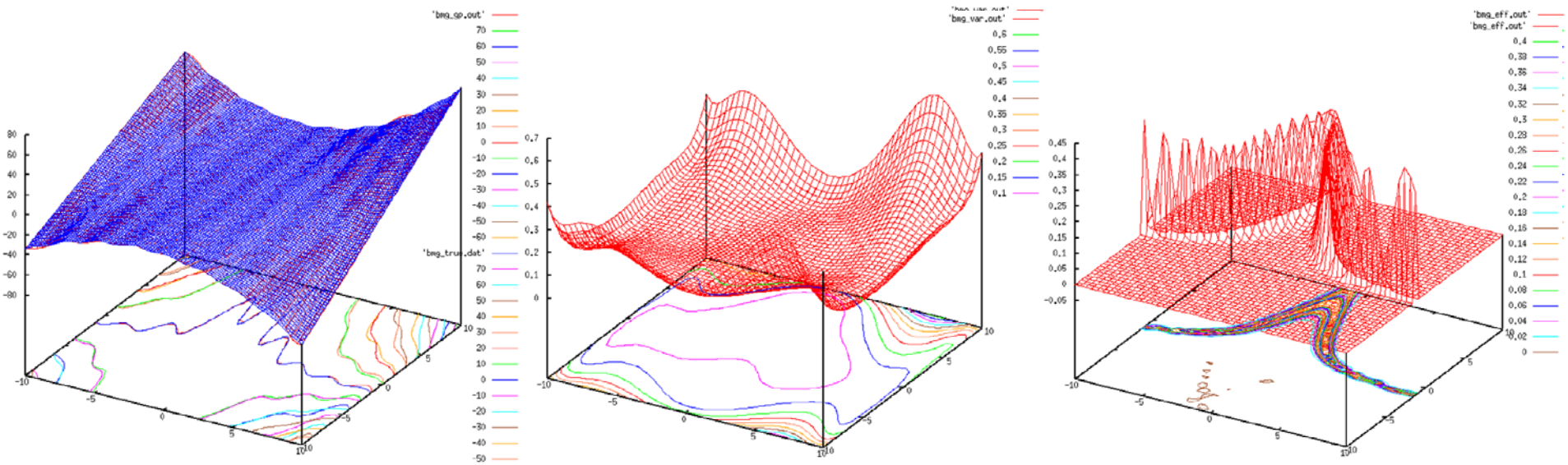
- Address known failure modes of local reliability methods:
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. fail to accurately estimate probability at MPP
- Based on EGO (surrogate-based global opt.), which exploits special features of GPs
  - Mean and variance predictions: formulate expected improvement (EGO) or expected feasibility (EGRA)
  - Balance explore and exploit in computing an optimum (EGO) or locating the limit state (EGRA)



From Jones, Schonlau, Welch, 1998

New UQ Method:
Efficient Global Reliability Analysis (EGRA)

- Address known failure modes of local reliability methods:
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. fail to accurately estimate probability at MPP
- Based on EGO (surrogate-based global opt.), which exploits special features of GPs
  - Mean and variance predictions: formulate expected improvement (EGO) or expected feasibility (EGRA)
  - Balance explore and exploit in computing an optimum (EGO) or locating the limit state (EGRA)

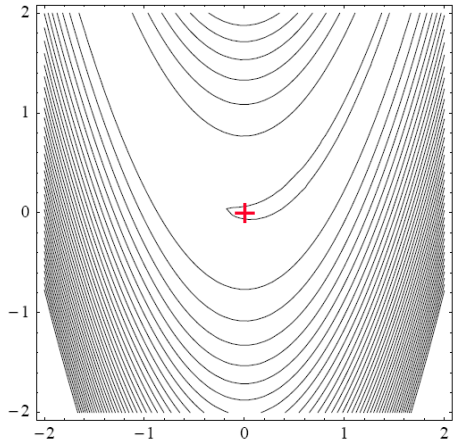


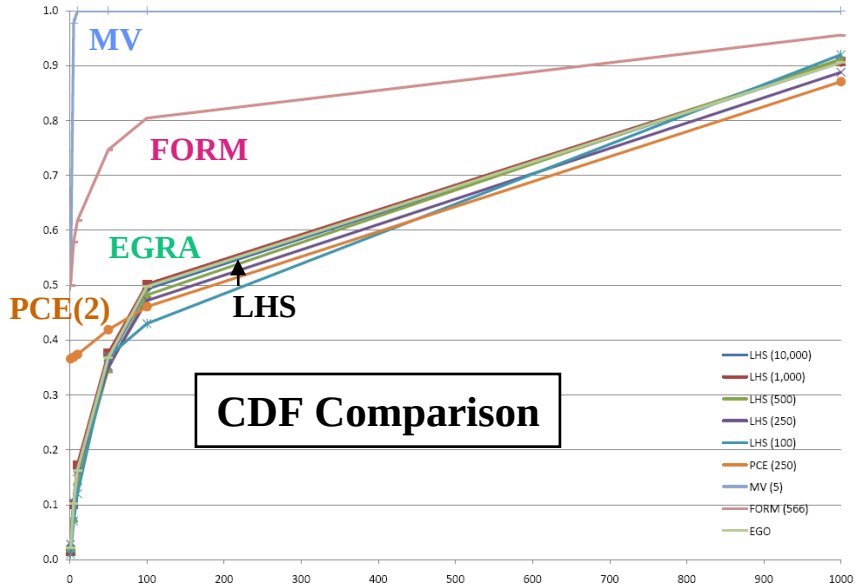
Accurate and efficient global estimation of failure surfaces

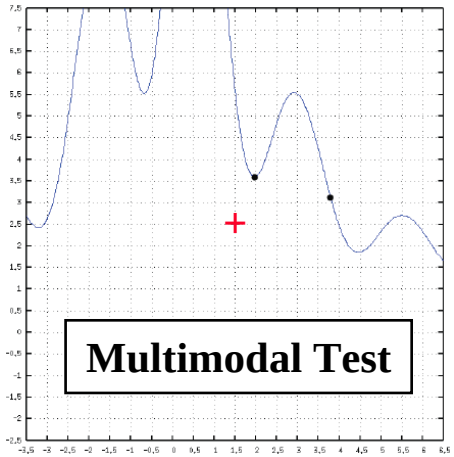
Sandia National Laboratories

EGRA (cont.): Benchmark performance

Rosenbrock Test







Reliability Method	Function Evaluations	First-Order p_f (% Error)	Second-Order p_f (% Error)	Sampling p_f (% Error, Avg. Error)
No Approximation	70	0.11797 (277.0%)	0.02516 (-19.6%)	—
x-space AMV^2+	26	0.11797 (277.0%)	0.02516 (-19.6%)	—
u-space AMV^2+	26	0.11777 (277.0%)	0.02516 (-19.6%)	—
u-space TANA	131	0.11797 (277.0%)	0.02516 (-19.6%)	—
LHS solution	10k	—	—	0.03117 (0.385%, 2.847%)
LHS solution	100k	—	—	0.03126 (0.085%, 1.397%)
LHS solution	1M	—	—	0.03129 (truth , 0.339%)
x-space EGRA	35.1	—	—	0.03134 (0.155%, 0.433%)
u-space EGRA	35.2	—	—	0.03133 (0.136%, 0.296%)

Accuracy similar to exhaustive sampling at cost similar to local reliability assessment

Generalized Polynomial Chaos Expansions

Approximate response w/ spectral proj. using orthogonal polynomial basis fns

e.g. $$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi})$$ using

$$\begin{aligned}
\Psi_0(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_0(\xi_2) &&= 1 \\
\Psi_1(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_0(\xi_2) &&= \xi_1 \\
\Psi_2(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_1(\xi_2) &&= \xi_2 \\
\Psi_3(\boldsymbol{\xi}) &= \psi_2(\xi_1)\,\psi_0(\xi_2) &&= \xi_1^2 - 1 \\
\Psi_4(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_1(\xi_2) &&= \xi_1\xi_2 \\
\Psi_5(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_2(\xi_2) &&= \xi_2^2 - 1
\end{aligned}$$

- Nonintrusive: estimate α_j using sampling (expectation), pt collocation (regression), tensor-product quadrature or Smolyak sparse grids (numerical integration)

Wiener-Askey Generalized PCE

- Tailor basis: optimal basis selection leads to exponential conv rates

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 $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0, \infty]$

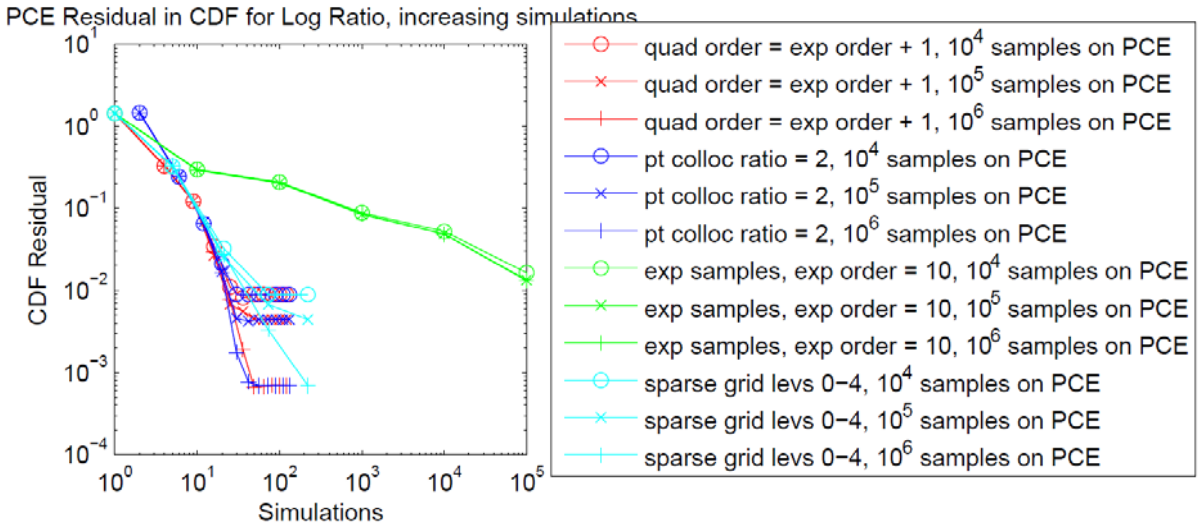
- Tailor expansion order/range: p/k-adaptivity based on PCE error estimation
  - Dimension p-refinement: anisotropic quadrature & Smolyak sparse grids
  - Dimension k-refinement: discretization of random domain

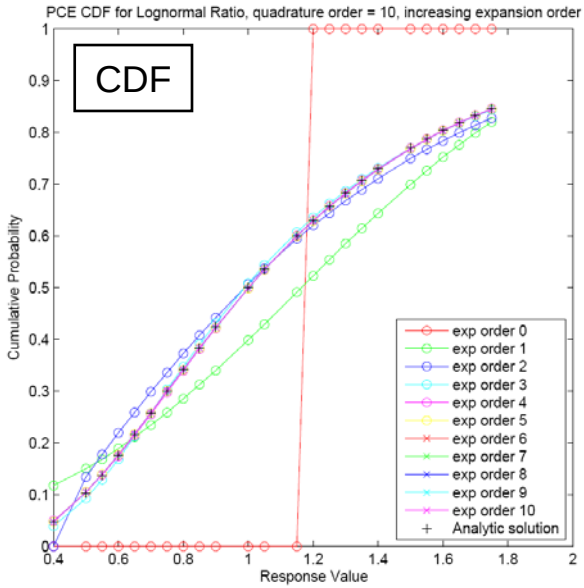
Sandia National Laboratories

Generalized PCE (cont.): Benchmark performance

Nonoptimal basis:

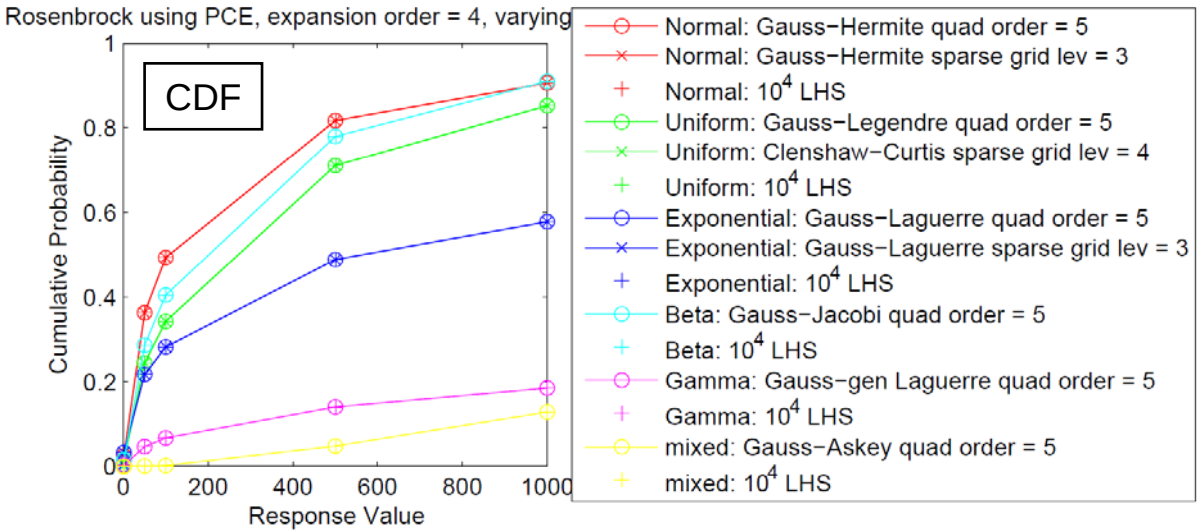
Hermite PCE for lognormals converges super-algebraically





Optimal basis:

Askey PCE for Rosenbrock is exact with 4th order expansion



Stochastic Collocation

Instead of estimating coeffs for known basis fns, form interpolants for known coeffs

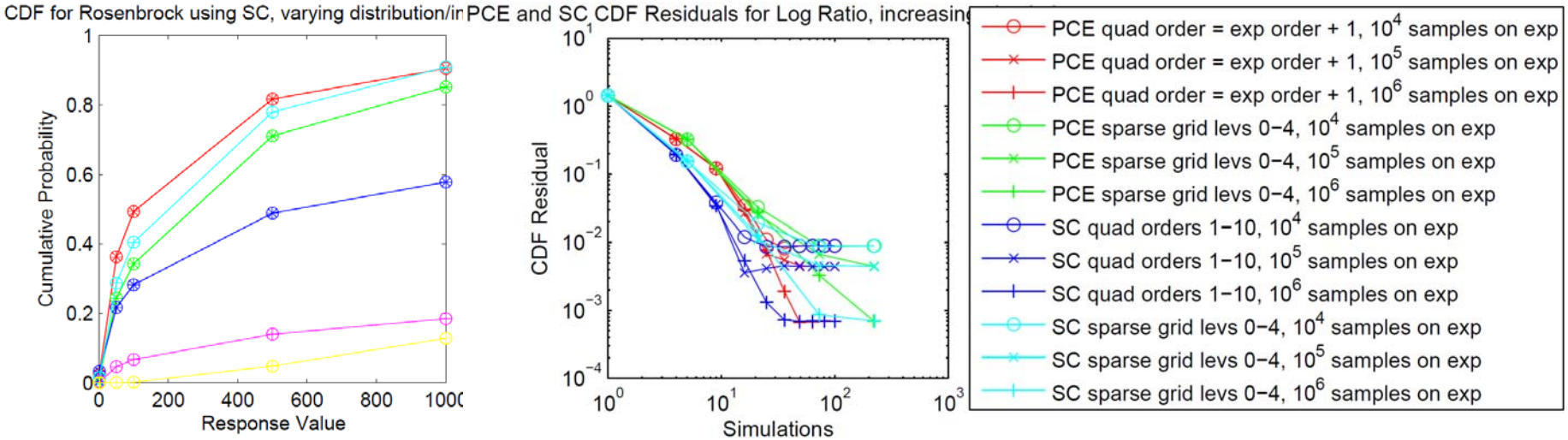
$$R = \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

$$L_i = \prod_{\substack{j=1 \\ j \neq i}}^{m} \frac{x - x_j}{x_i - x_j}$$

Key is use of same quadrature or sparse grid points/weights from the orthogonal polynomials for specified input PDFs → same exponential convergence rates

Advantages relative to PCE: **Simpler (no expansion order), adapts to integration pt set (doesn't over-/under-integrate expansion), easy moment estimation, no intrusive variant**

Disadvantages relative to PCE: **Formation of interpolant (for CDF sampling) requires structured data sets: quadrature/sparse grid (only); approx. error not orthogonal to basis**



PCE Example

- Compare stochastic expansion methods to other UQ methods considered thus far (examples/methods/dakota_pce.in)

Example Input/Output: PCE

```
strategy,
    single_method

method,
            nond_polynomial_chaos
              expansion_order    = 4 2
              quadrature_order   = 5 3
              samples = 10000
              seed    = 12347
              response_levels =
              .1 1. 50. 100.
              500. 1000.

variables,
            uniform_uncertain = 2
              lower_bounds      = -2.  -2.
              upper_bounds      =  2.   2.
              descriptors       = 'x1' 'x2'

interface,
            direct
            analysis_driver = 'rosenbrock'
responses,
            num_response_functions = 1
            no_gradients
            no_hessians
```

PCE Input (examples/methods/dakota_pce.in)

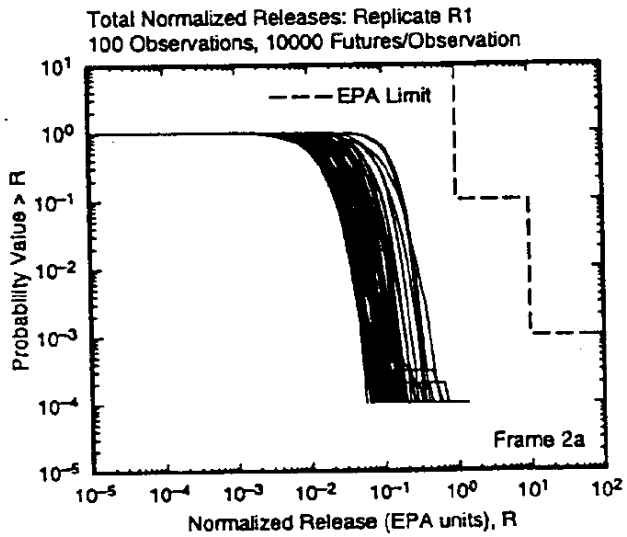
```
<<<<< Function evaluation summary: 15 total (15 new, 0 duplicate)
Polynomial Chaos coefficients for response_fn_1:
      coefficient   u1   u2
      ----------- ---- ----
  4.5566666667e+02   P0   P0
 -4.0000000000e+00   P1   P0
  9.1695238095e+02   P2   P0
...
Statistics derived analytically from polynomial expansion:
Moments for each response function:
response_fn_1:  Mean = 4.5566666667e+02  Std. Dev. = 6.0656024184e+02  Coeff.
of Variation = 1.3311490311e+00

Sensitivities for each response function evaluated at uncertain variable means:
response_fn_1:   [ -2.0000000000e+00  2.4505397711e-13 ]

Statistics based on 10000 samples performed on polynomial expansion:
Probabilities for each response function:
Cumulative Distribution Function (CDF) for response_fn_1:
    Response Level  Probability Level  Reliability Index  General Rel Index
    --------------  -----------------  -----------------  -----------------
  1.0000000000e-01   1.9000000000e-03
  1.0000000000e+00   1.3600000000e-02
  5.0000000000e+01   2.4390000000e-01 ...
```

PCE Output

Epistemic UQ

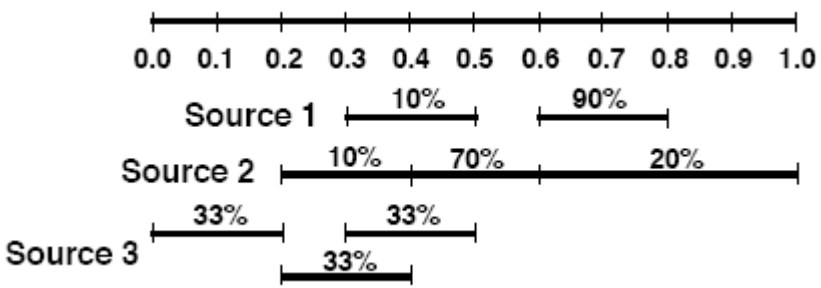
Second-order probability

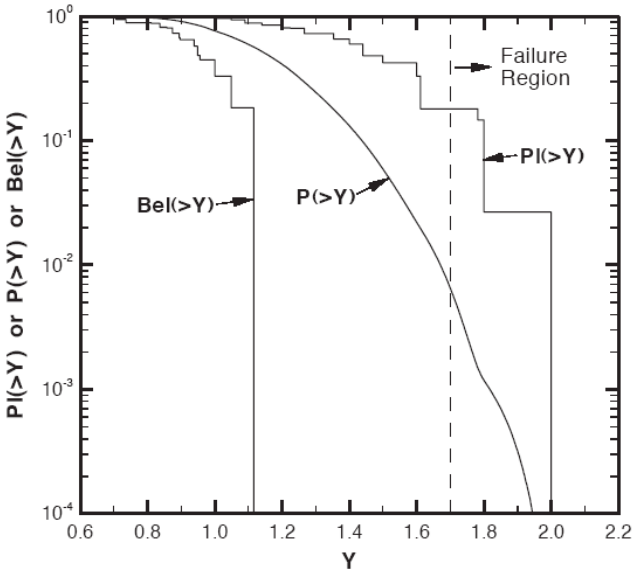
- Two levels: distributions/intervals on distribution parameters
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).



Dempster-Shafer theory of evidence

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

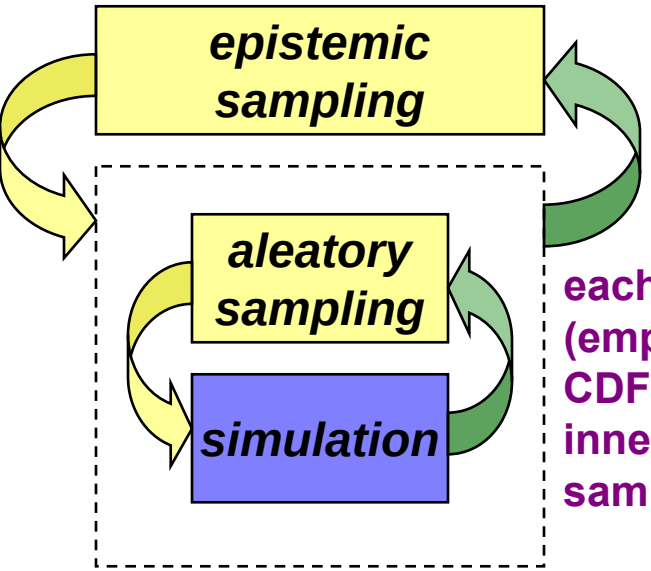




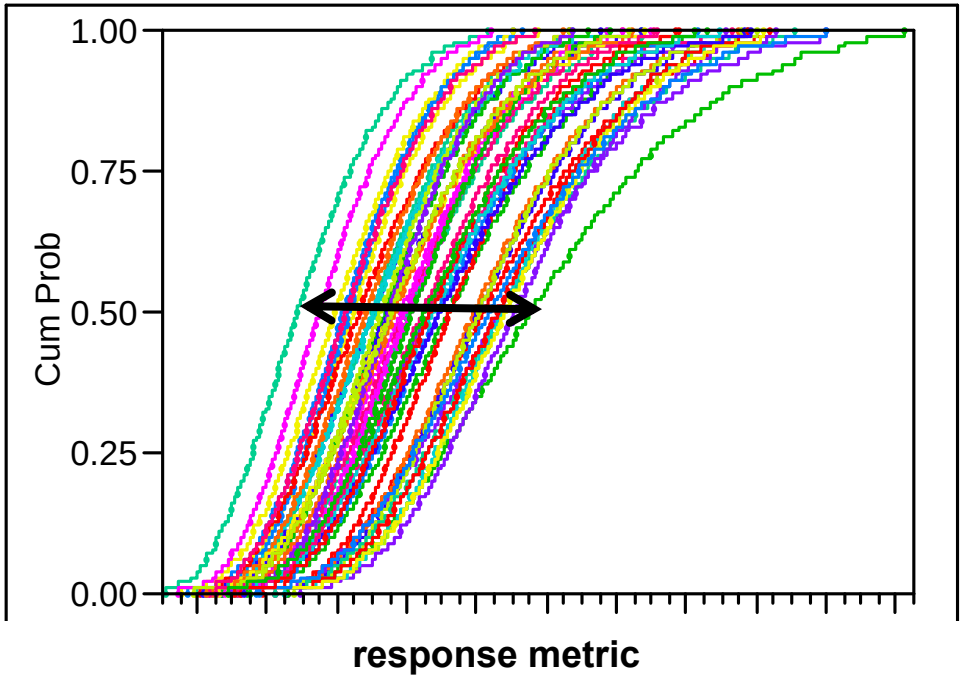
Second-order Probability

- **For each outer loop sample of epistemic (interval) variables, run an inner loop UQ study over aleatory (probability) variables**

50 outer loop samples
→ 50 CDF traces

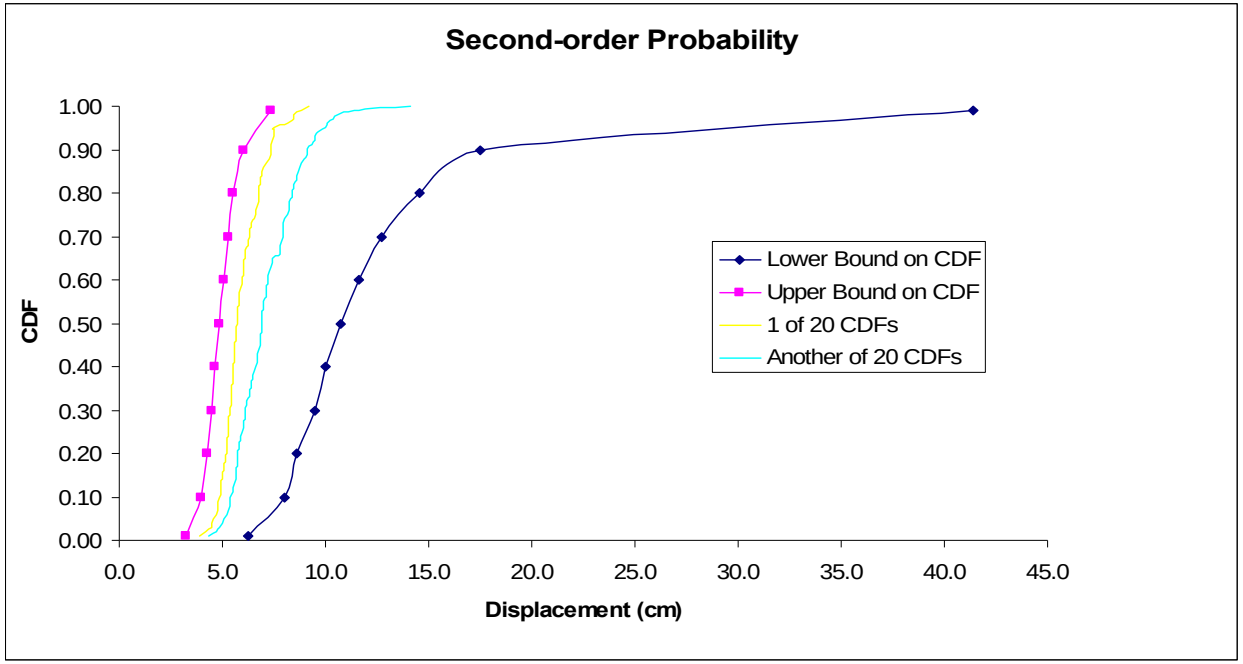


each discrete (empirical) CDF: 100 inner loop samples



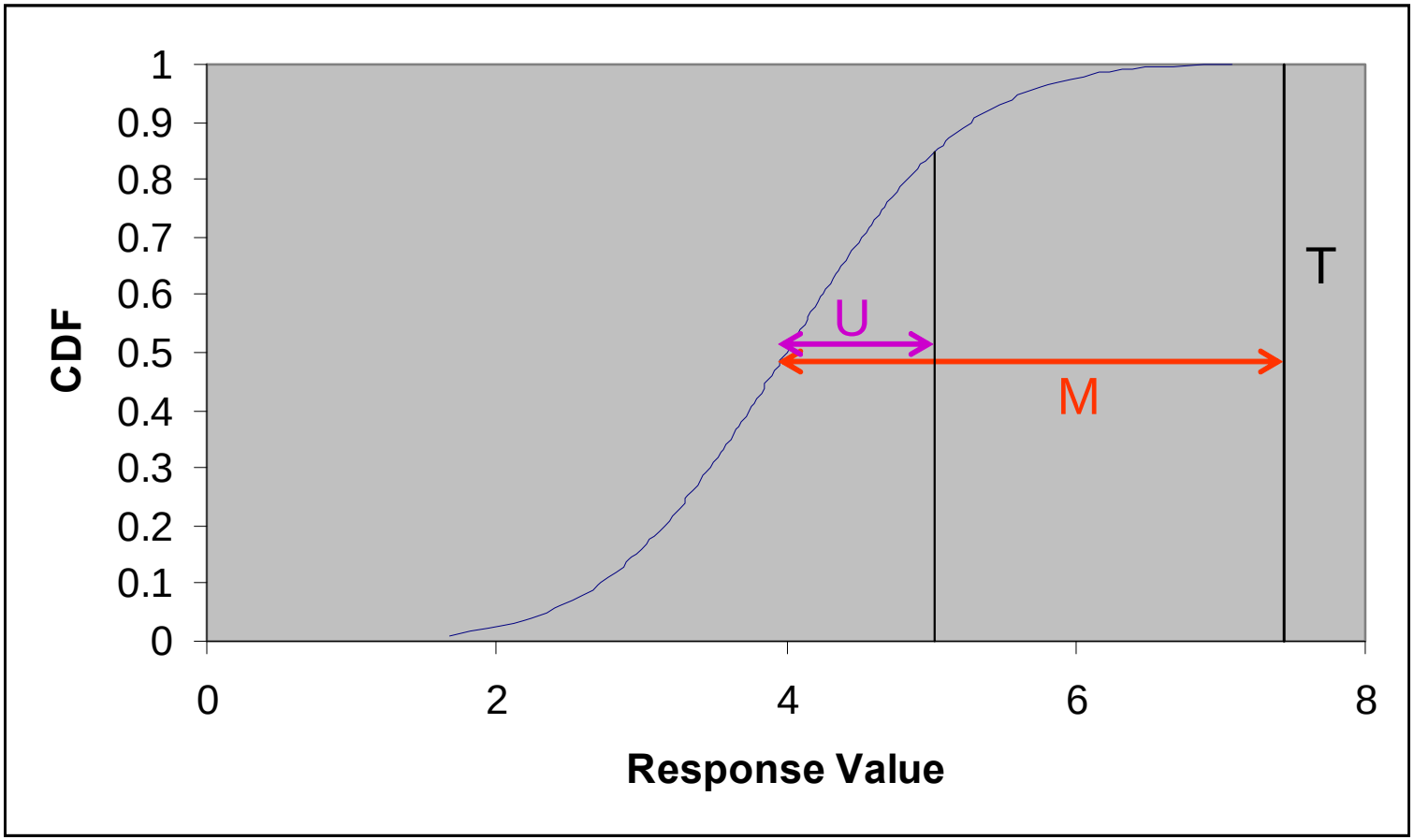
"Envelope" of CDF traces represents response epistemic uncertainty

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

QMU Example

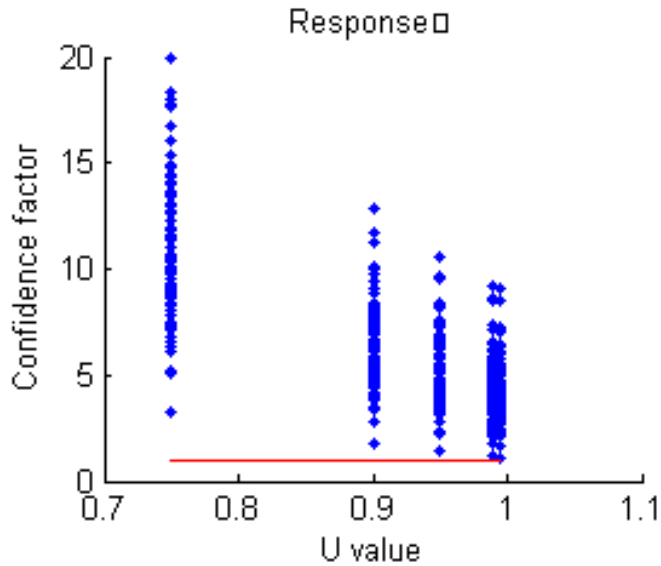


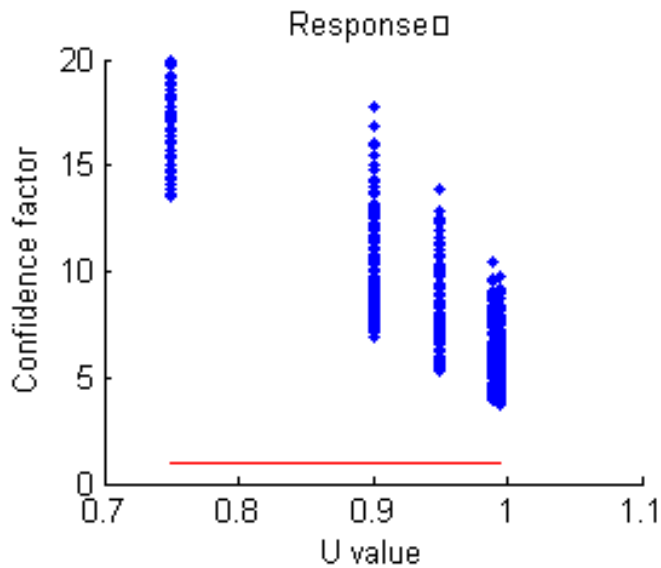
$$CF = M/U$$

QMU Example

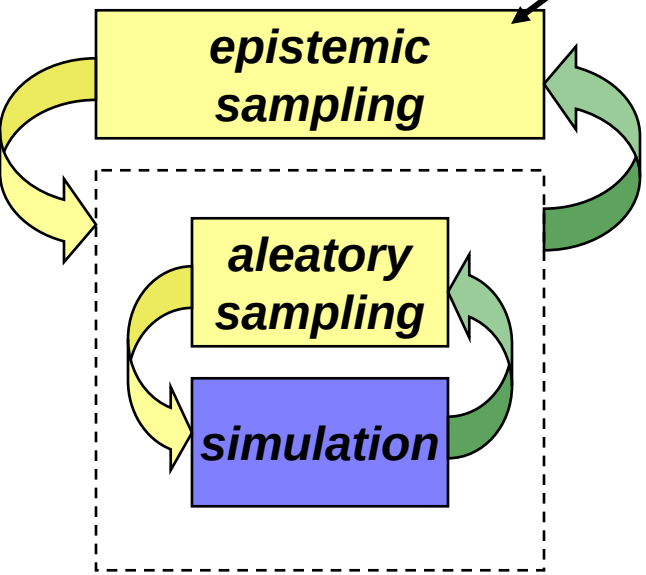
- Typical standard case:
  - Create N samples on inputs, run code N times, generate a CDF of output metric
  - Calculate M, U, and CF based on the CDF and the threshold
- Other cases:
  - Uncertainty in both response and threshold
  - Intervals on both response and threshold
  - Interval bounds on threshold, evidence theory or probability representation of response
  - Evidence theory or probabilistic representation of both response and threshold

QMU Example


Response
Confidence factor
U value
0
5
10
15
20
0.7
0.8
0.9
1
1.1


Response
Confidence factor
U value
0
5
10
15
20
0.7
0.8
0.9
1
1.1

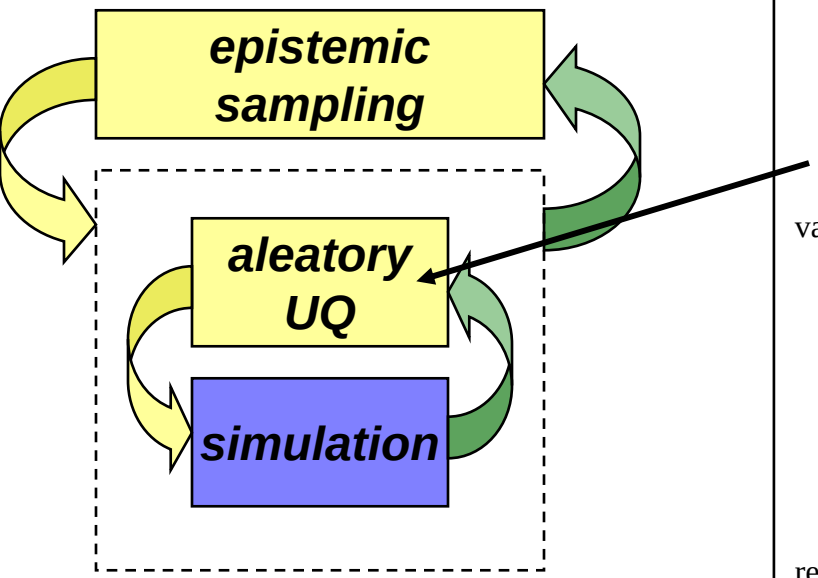
Example Input: Second-Order Probability




```
method,
                id_method = 'EPISTEMIC'
                model_pointer = 'EPIST_M'
                nond_sampling   samples = 50 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. 1. 0. 0. 0
                                              0. 0. 0. 0. 0. 0. 0. 1.
variables,
                id_variables = 'EPIST_V'
                interval_uncertain =2
                 num_intervals = 1 1
                 interval_probs = 1.0 1.0
                 interval_bounds = 400. 600. 800. 1200.
                 descriptors       'X_mean' 'Y_mean'

responses,
                id_responses = 'EPIST_R'
                num_response_functions = 3
                response_descriptors = 'mean_wt' 'ccdf_beta_s' 'ccdf_beta_d'
```

PCE Input (examples/methods/dakota_uq_cantilever_2nd_order.in)

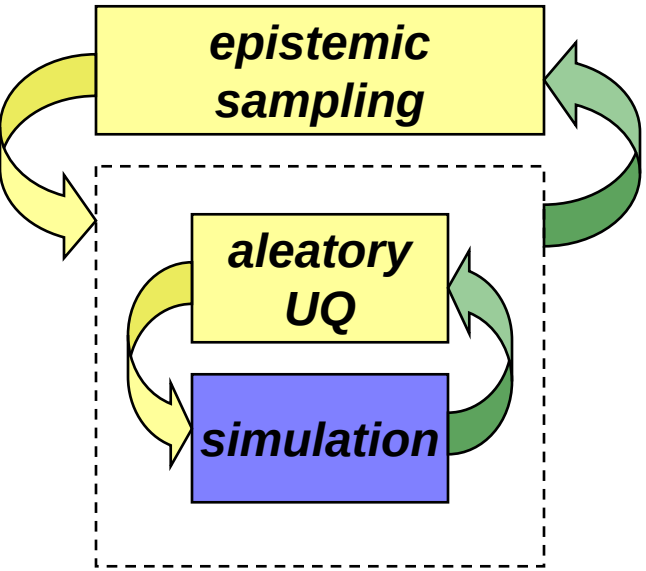
Example Input: Second-Order Probability




```
method,
                id_method = 'ALEATORY'
                model_pointer = 'ALEAT_M'
                nond_local_reliability
                  mpp_search no_approx
                  num_response_levels = 0 1 1
                  response_levels = 0.0 0.0
                  compute reliabilities  complementary distribution
model,
                id_model = 'ALEAT_M'
                single
                  variables_pointer = 'ALEAT_V'
                  interface_pointer = 'ALEAT_I'
                  responses_pointer = 'ALEAT_R'

variables,
                id_variables = 'ALEAT_V'
                continuous_design = 2
                  initial_point    2.4522 3.8826
                  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,
                id_responses = 'ALEAT_R'
                num_response_functions = 3
                response_descriptors = 'weight' 'stress' 'displ'
```

PCE Input (examples/methods/dakota_uq_cantilever_2nd_order.in)

Example Output: Second-Order Probability




```
<<<<< 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
      ....
```

PCE Input (examples/methods/dakota_uq_cantilever_2nd_order.in)

UQ 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	(10-30) * M Note: the number of samples depends on the statistics of the output distribution being resolved.	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

Extra Slides

More Detail: Uncertainty Quantification Methods

- Latin Hypercube sampling
- Analytic reliability methods
- Polynomial chaos expansions
- Dempster-Shafer theory of evidence
- "Second-order" probability analysis

- Aleatory
  - Inherent variability (e.g., in a population)
  - Irreducible uncertainty – can't reduce it by further knowledge
- Epistemic
  - Subjective uncertainty
  - Related to what we don't know
  - Reducible: If you had more data or more information, you could make your uncertainty estimation more precise

Introduction

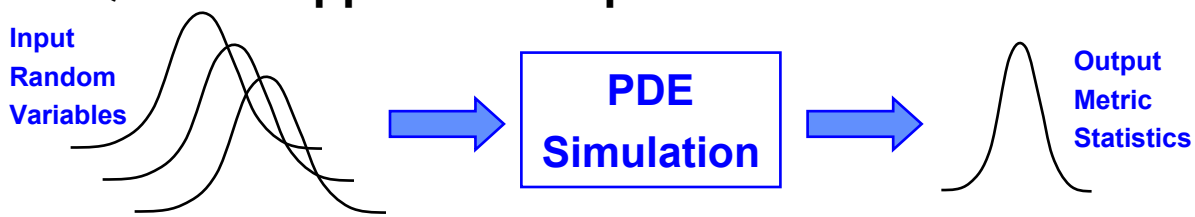
Uncertainties/variabilities must be properly modeled in order to quantify risk and design systems that are robust and reliable

Uncertainty can be categorized to be one of two different types:

- **Aleatory/irreducible: inherent variability with sufficient data → probabilistic models**
- **Epistemic/reducible: uncertainty from lack of knowledge → nonprobabilistic models**

  Harder problem

We use a UQ-based approach to optimization under uncertainty (OUU)

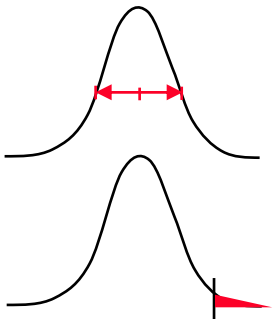


- **safety factors, multiple operating conditions, or local sensitivities are insufficient**
- **focus is simulation-based engineering apps: large-scale PDE-based, transient, nonlinear, implicit (distinct from chance-constrained stochastic programming – often linear/explicit)**
- **tailor OUU methods to strengths of different UQ approaches**

OUU methods encompass both:

- **design for robustness (moment statistics: mean, variance)**
- **design for reliability (tail statistics: probability of failure)**

  Harder problem



Background on V&V/UQ

- **Verification**
  - **Are you solving the equations correctly?**
  - **Code verification: SQE, especially unit/regression/verification testing**
    - **Algorithms of interest: method of manufactured solutions**

$$p = \frac{1}{\ln r} \ln\left(\frac{E_{grid1}}{E_{grid1}}\right)$$

  - **Solution verification: spatial/temporal/iterative convergence of results**
    - **Algorithms of interest: Richardson extrapolation, Finite element error estimation (ZZ, QOI)**

$$\eta^Q \equiv \int_\Omega \boldsymbol{T}(\boldsymbol{u}_h) : (\boldsymbol{G}(\boldsymbol{\nabla} \boldsymbol{z}_h) - \boldsymbol{\nabla} \boldsymbol{z}_h)\, \mathrm{d}\Omega$$

- **Validation**
  - **Are you solving the correct equations?**
    → Assessment of computational models for intended application domains
  - **Compare** [simulation + sim. uncertainty] **vs.** [experimental + data uncertainty]
  - **Validation is hierarchical: material tests → components → subsys → sys**
  - **Validation is targeted: models are validated for particular apps in particular regimes**
  - **UQ is an enabling tool for validation**
- **SNL/LANL/LLNL have large V&V programs as part of ASC**
  - **QMU initiative for decision support: ratio of margin/uncertainty should be > 1**

Sampling Capabilities

Motivations:

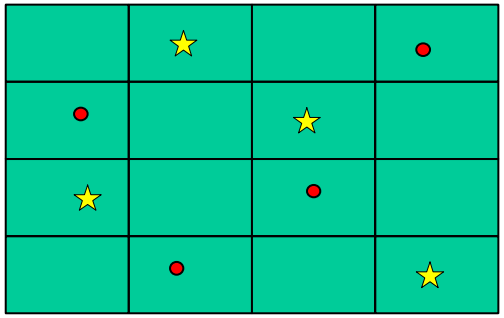
- Surrogates: Data fit, spanning ROM
- UQ

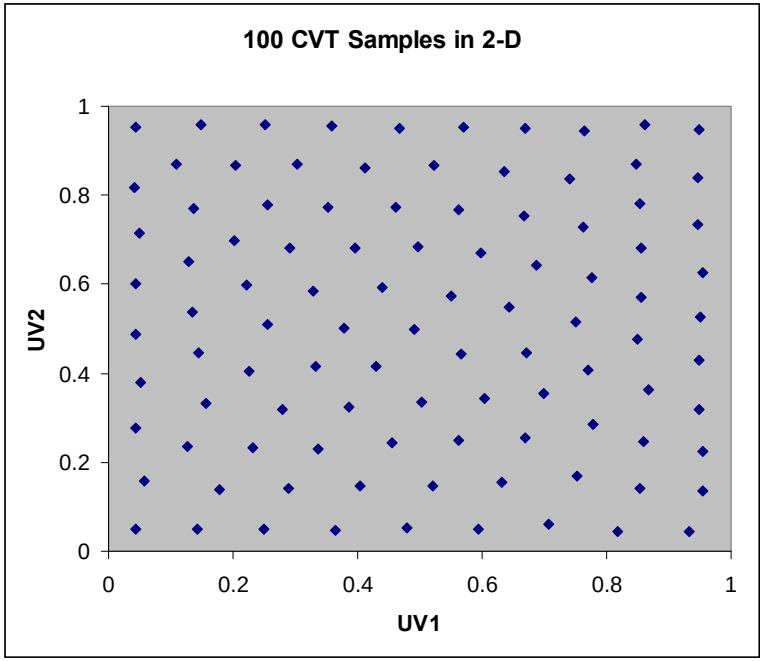
Types:

- Monte Carlo: basic random sampling
- Pseudo Monte Carlo: Latin Hypercube Sampling (LHS) is a stratified, structured sampling method that picks random samples from equal probability bins for all 1-D projections.
- Quasi Monte Carlo: deterministic sequences constructed to uniformly cover a unit hypercube with low discrepancy.
  E.g., Halton, Hammersley, Sobol
- Centroidal Voronoi Tesselation (CVT): generates nearly uniform spacing over arbitrarily shaped parameter spaces; originally developed for "meshless" mechanics methods.
- (Multimodal, Adaptive) Importance Sampling: generates samples with recentered density to emphasize areas of importance (i.e., tails)

Associated Tools:

- Volumetric quality, Latinization
- Correlations, variance-based decomposition





RBDO Algorithms

Bi-level RBDO

- **Constrain RIA *z* → *p*/*β* result**
- **Constrain PMA *p*/*β* → *z* result**

RIA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \beta \geq \bar{\beta} \\ \text{or} & p \leq \bar{p} \end{cases}$$

PMA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & z \geq \bar{z} \end{cases}$$

Fully analytic Bi-level RBDO

- **Analytic reliability sensitivities avoid numerical differencing at design level**

$$\begin{cases} \nabla_{\mathbf{d}} z = \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} \beta_{cdf} = \dfrac{1}{\| \nabla_{\mathbf{u}} G \|} \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} p_{cdf} = -\phi(-\beta_{cdf}) \nabla_{\mathbf{d}} \beta_{cdf} \end{cases}$$
(1st order)

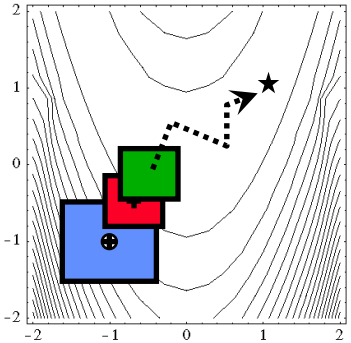
If **d** = distr param, then expand
$$\nabla_{\mathbf{d}} g = \nabla_{\mathbf{d}} \mathbf{x} \nabla_{\mathbf{x}} g$$

Sequential/Surrogate-based RBDO:

- **Break nesting: iterate between opt & UQ until target is met. Trust-region surrogate-based approach is non-heuristic.**

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{d}_0) + \nabla_d f(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \\ \text{subject to} \quad & \beta(\mathbf{d}_0) + \nabla_d \beta(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \geq \bar{\beta} \\ & \| \mathbf{d} - \mathbf{d}_0 \|_\infty \leq \Delta^k \end{aligned}$$

1st-order
(also 2nd-order w/ QN)



Unilevel RBDO:

- **All at once: apply KKT conditions of MPP search as equality constraints**
  - Opt. increases in scale (***d***,***u***)
  - Requires 2nd-order info for derivatives of 1st-order KKT

$$\begin{aligned} \min_{\mathbf{d}_{aug} = (\mathbf{d}, \mathbf{u}_1, .., \mathbf{u}_{N_{hard}})} & : f(\mathbf{d}, \mathbf{p}, \mathbf{y}(\mathbf{d}, \mathbf{p})) \\ \text{s. t.} \quad & : G_i^R(\mathbf{u}_i, \eta) = 0 \\ & \beta_{allowed} - \beta_i \geq 0 \\ & \|\mathbf{u}_i\| \, \|\nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i, \eta)\| + \mathbf{u}_i^T \nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i, \eta) = 0 \\ & \beta_i = \|\mathbf{u}_i\| \\ & \mathbf{d}^l \leq \mathbf{d} \leq \mathbf{d}^u \end{aligned}$$

KKT of MPP

Sandia National Laboratories

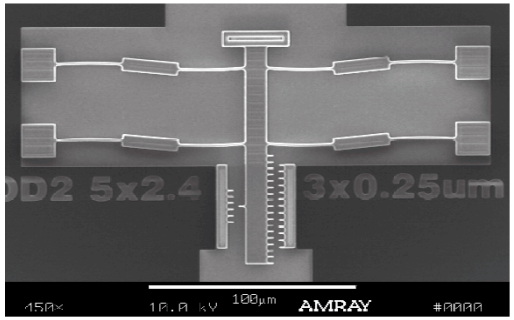
Shape Optimization of Compliant MEMS

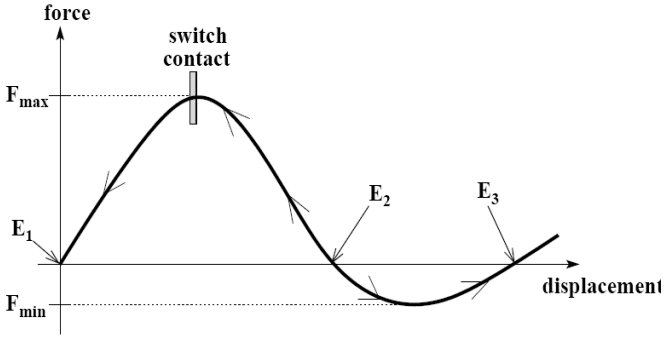
- **MEMS subject to substantial variabilities & lack historical knowledge base**
- **Sources of uncertainty**
  - **Material properties, manufactured geometries, residual stresses**
  - **Data can be obtained → aleatoric uncertainty, probabilistic approaches**
- **Resulting part yields can be low or have poor cycle durability**

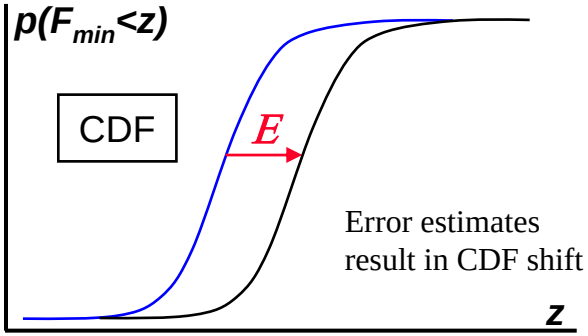
Solution-Verified Reliability Analysis & Design of MEMS

- **Account for both manufacturing uncertainties and simulation errors in MEMS design**
- **Integrate UQ/RBDO (DAKOTA), ZZ/QOI error est (Coda), adapt (SIERRA), nonlin mech (Aria) → MESA**
- **Goals: On-line soln verification → project UQ/OUU results to fully converged mesh; Achieve prescribed reliability; Minimize sensitivity to uncertainties (robustness)**

Bi-stable MEMS Switch

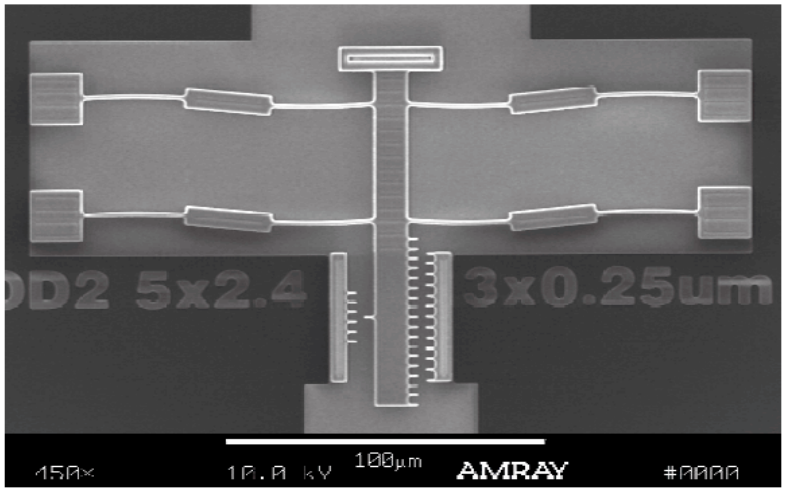


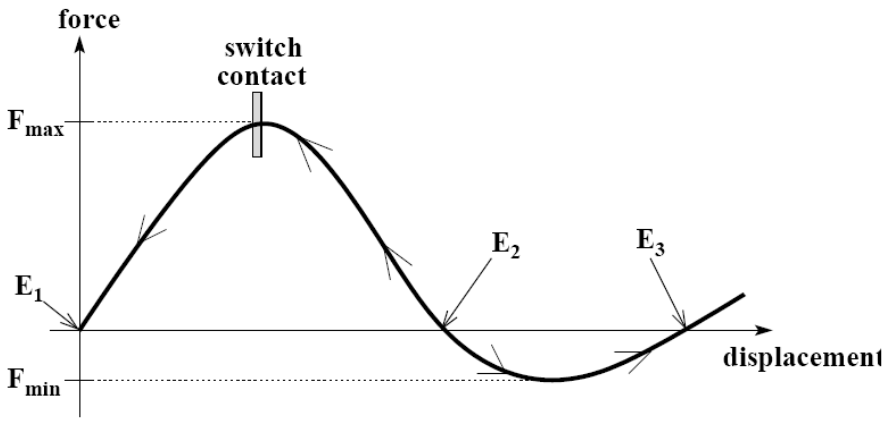


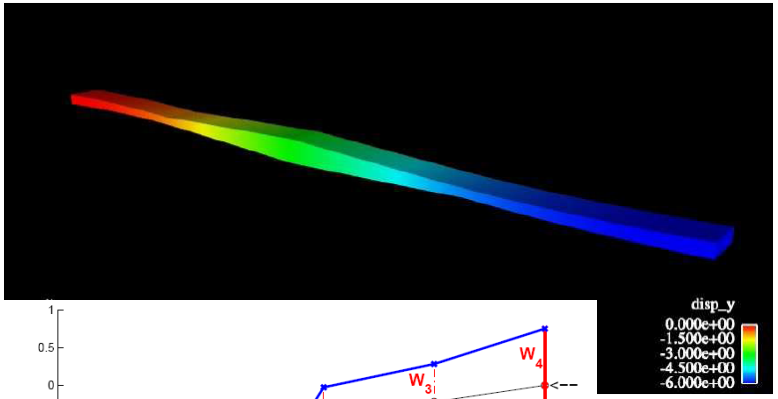


- ➢ ***Error-corrected***: **EE as analysis correction factors**
- ➢ ***Error-informed***: **EE as indicators for uniform/adaptive refinement (tight tols: eliminate correction)**
- ➢ ***Combined***: **control error levels (loose tols: assure correction accuracy) & use correction factors**

Bi-Stable Switch: Problem Formulation







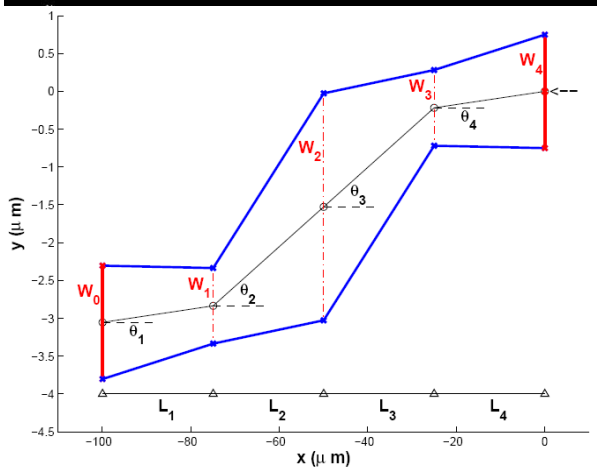
13 design vars: W_i, L_i, θ_i

2 random vars:

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

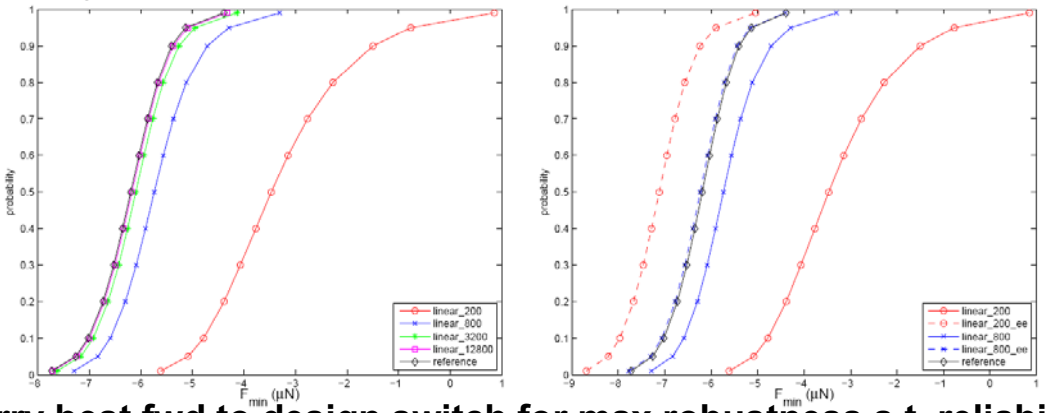
$$
\begin{array}{llcl}
\max & & & F_{min}(\mathbf{d}, \mu) \\
\text{s.t.} & 2 & \leq & \beta(\mathbf{d}) \\
 & 50 & \leq & F_{max}(\mathbf{d}, \mu) \leq 150 \\
 & & & E_2(\mathbf{d}, \mu) \leq 8 \\
 & & & S_{max}(\mathbf{d}, \mu) \leq 1200
\end{array}
$$

→ **reliable + robust**

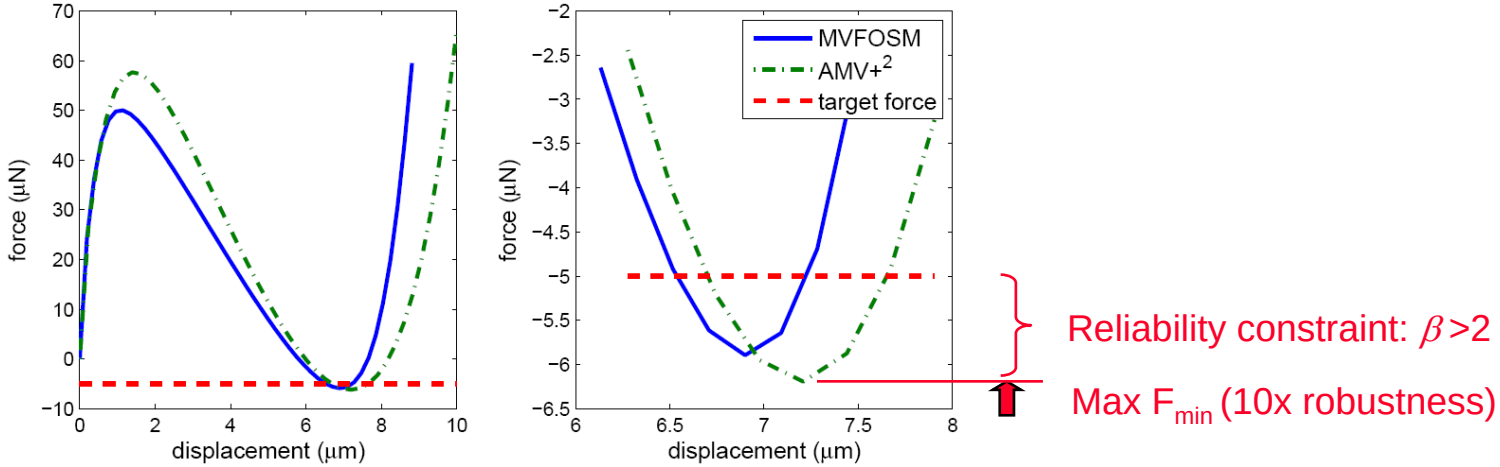


Results:
Solution-Verified Reliability Analysis and Design

- **Reliability analysis: compute error-corrected CDFs and assess accuracy/efficiency**



- **RBDO: carry best fwd to design switch for max robustness s.t. reliability constraint**



Conclusions: **UQ/OUU with error corrected/informed approaches can be:**

- **more accurate: controlling/correcting errors leads to higher confidence in UQ/RBDO results**
- **less expensive: `Linear800+EE` analysis above < 10% cost of fully converged reference**
- **more reliable: on-line approach accounts for any parameter dependence (esp. shape vars)**
- **more convenient: can eliminate need for manual *a priori* convergence studies**

Sandia National Laboratories

Adding Samples

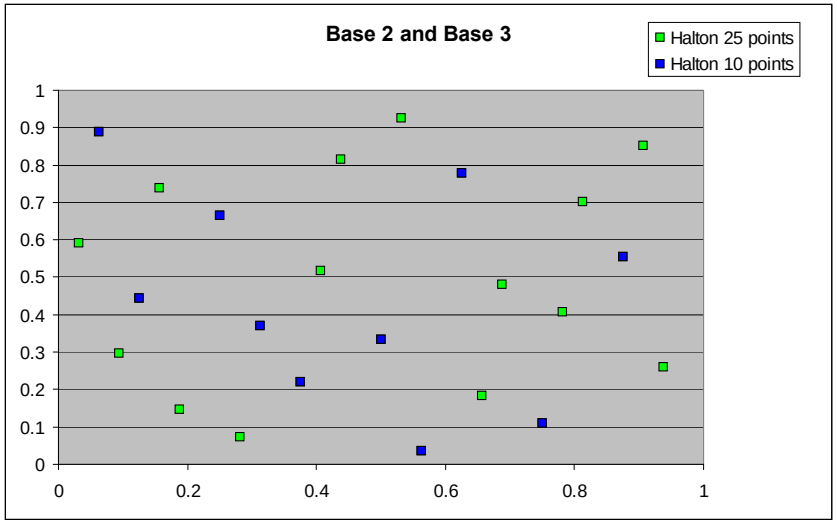
- The Halton Quasi Monte Carlo sampling method allows you to add one sample at a time
- LHS does not: As you go from 50 to 51 samples, 51 samples requires a restratification of the input space to 51 bins, and new samples
- However, we have an "incremental" LHS sampling capability
- Using this approach, we can double the number of LHS samples each time, maintaining both the correlation structure and the proper stratification
- Use incremental LHS to go from 20 to 40 to 80 samples, etc.
- Must have a restart file with the previous run available
- Syntax:
  - samples = 20
  - seed = 234
  - sample_type incremental_lhs previous_samples = 10

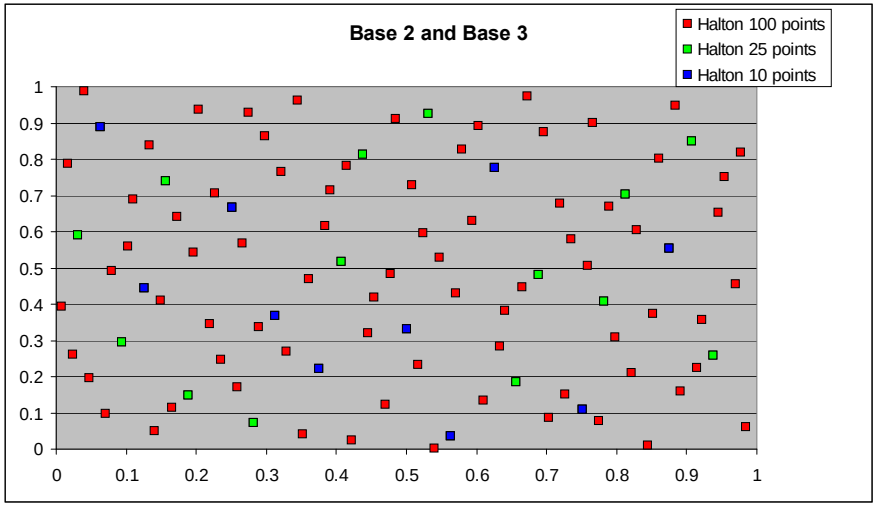
Quasi Monte Carlo Methods

- **Quasi-Monte Carlo sequences are deterministic sequences determined by a series of prime bases. They are designed to produce uniform random numbers on the interval [0,1].**
- **E.g., Halton sequence:**

Sample Number	Base 2	Base 3	Base 5	Base 7
1	0.5000	0.3333	0.2000	0.1429
2	0.2500	0.6667	0.4000	0.2857
3	0.7500	0.1111	0.6000	0.4286
4	0.1250	0.4444	0.8000	0.5714
5	0.6250	0.7778	0.0400	0.7143
6	0.3750	0.2222	0.2400	0.8571
7	0.8750	0.5556	0.4400	0.0204
8	0.0625	0.8889	0.6400	0.1633
9	0.5625	0.0370	0.8400	0.3061
10	0.3125	0.3704	0.0800	0.4490

Example: Halton Set

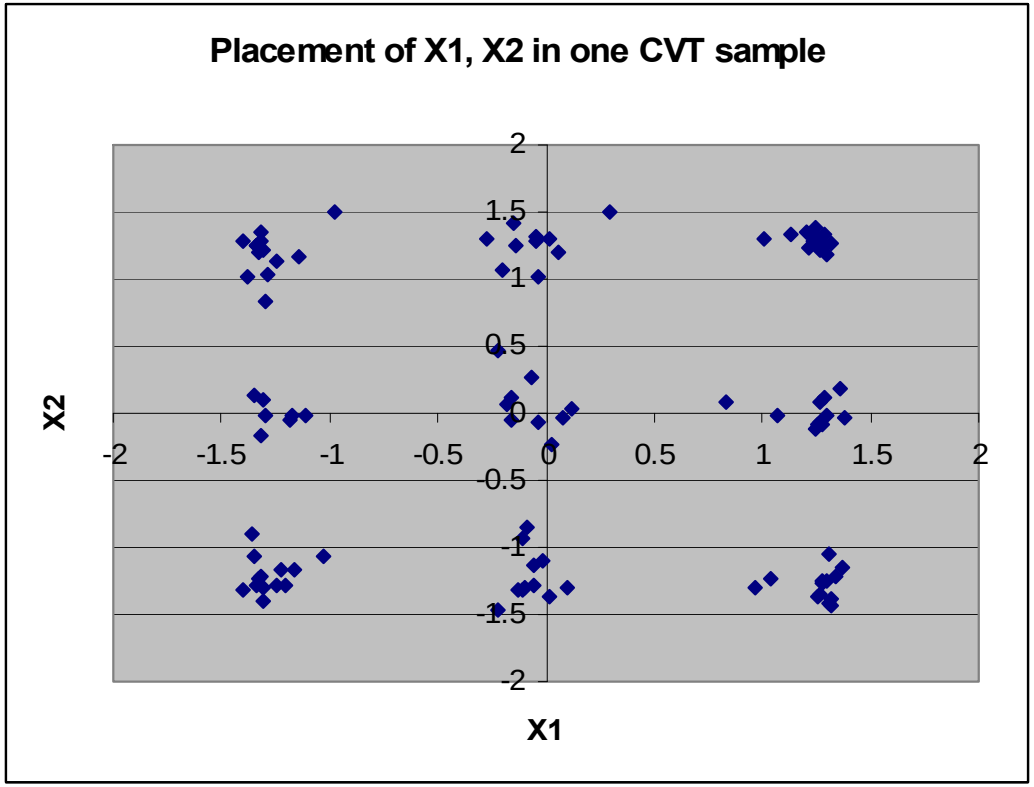




Quasi Monte Carlo Methods

- The quasi-Monte Carlo (QMC) and Centroidal Voronoi Tesselation (CVT) methods are designed with the goal of low discrepancy.
- Discrepancy refers to the nonuniformity of the sample points within the hypercube.
- Low discrepancy sequences tend to cover the unit hypercube reasonably uniformly.
- CVT does very well volumetrically, however the lower-dimension (such as 1-D) projections of CVT can have high discrepancy.
- CVT developed as part of unstructured meshing techniques for irregular domains
- Centroidal Voronoi diagrams subdivide arbitrarily shaped domains into arbitrary numbers of nearly uniform subvolumes
- Sample points returned are the centers of the Voronoi region
- CVT good choice for high dimensional sampling

CVT Performance

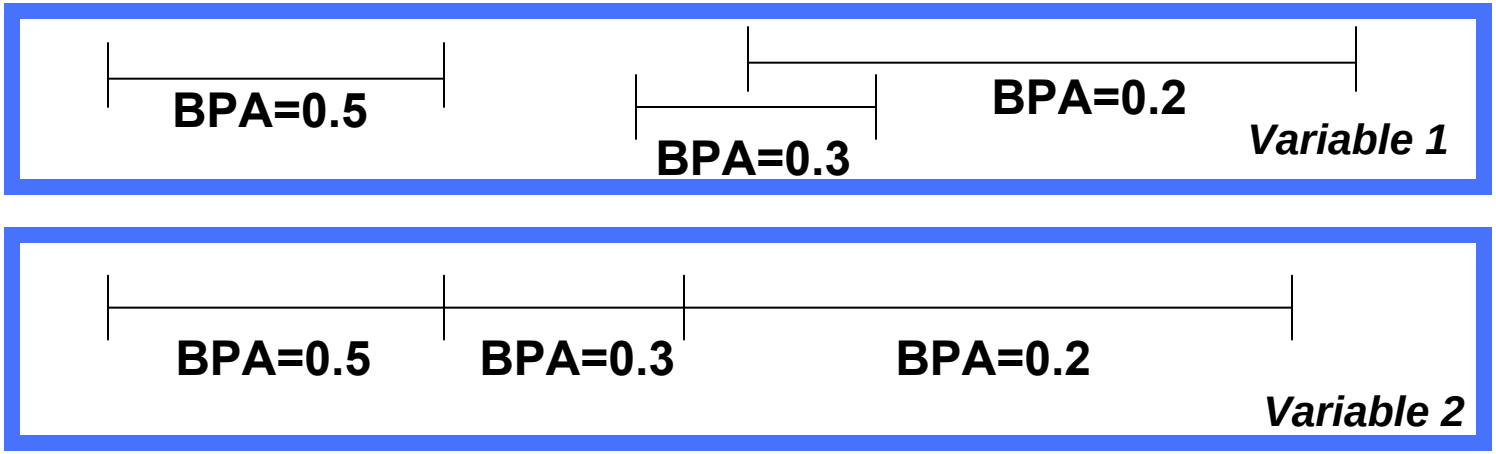


•This clustering may contribute to the method performing relatively well over all the space but poorly at the edges, which the RMSE metric emphasizes.

•Note that there is an approach which “latinizes” or stratifies the CVT samples to give them better 1-D marginal densities, which may improve their potential use in response surface modeling.

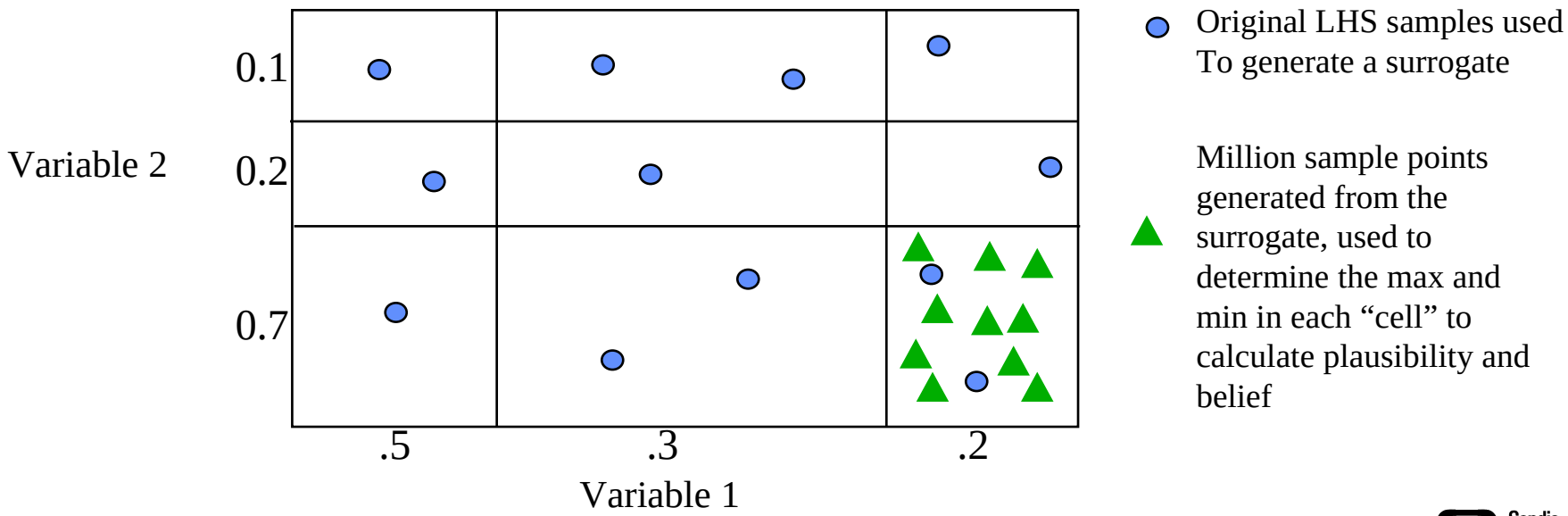
Epistemic Uncertainty Quantification

- 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"



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

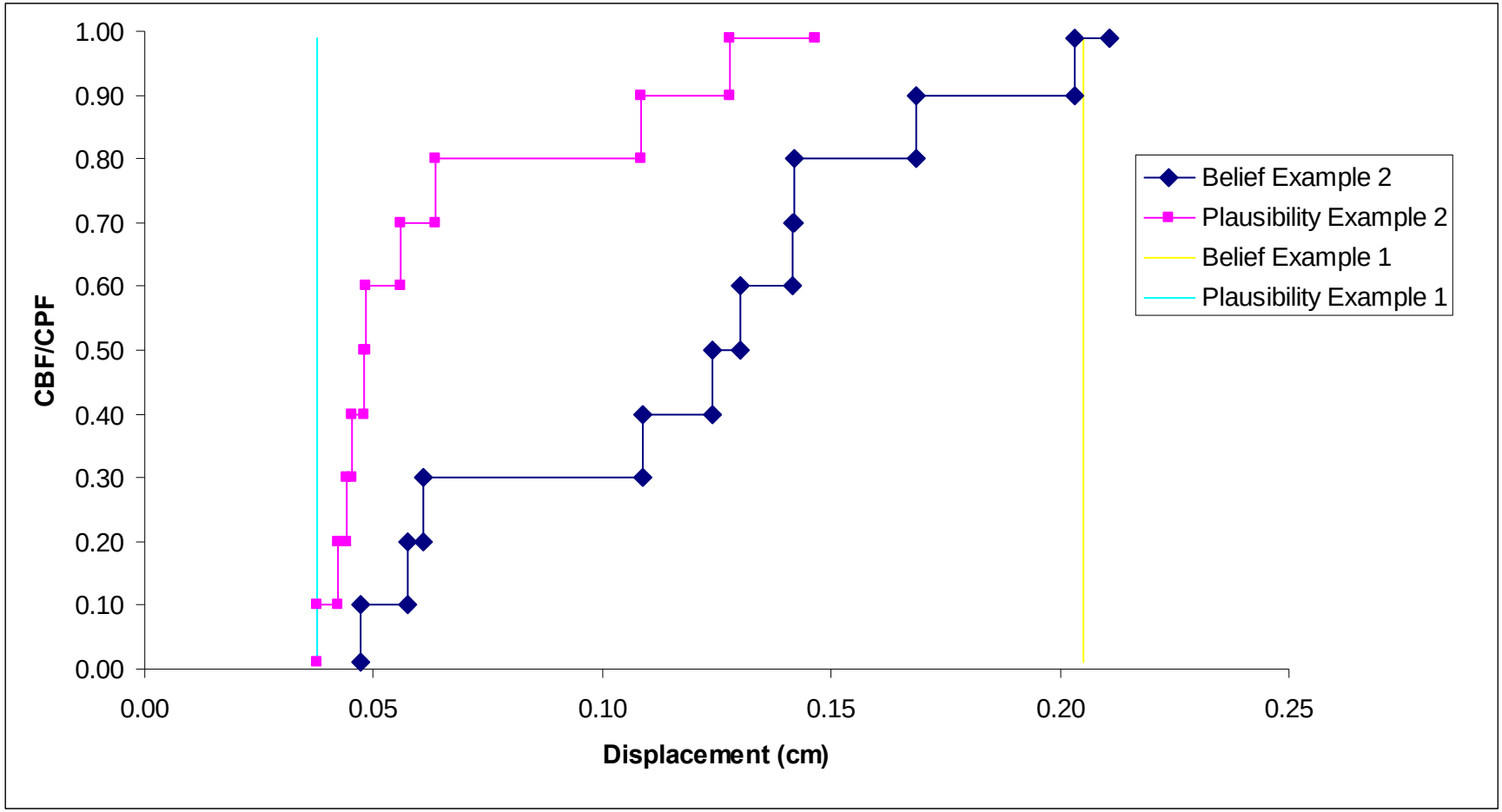


Dempster-Shafer Example

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