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DAKOTA
and its use in Computational Experiments

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Outline/Agenda

- DAKOTA history and background
- DAKOTA methods
  - Parameter study
  - Uncertainty quantification
  - Optimization
- DAKOTA input/output/script files
- Uncertainty Quantification
  - Design of Computer Experiments
  - Analytic Reliability Methods
  - Epistemic Uncertainty
- Engineering applications

What is DAKOTA? Executive Summary

- DAKOTA: Design and Analysis toolKit for Optimization and Terascale Applications
  - Under development at SNL since 1994
  - State of the art tools for performing engineering "what if" studies:
    - Uncertainty quantification, sensitivity analysis, computer model calibration, design optimization, etc.
    - Extensive support for parallel computing – PCs to supercomputers
  - Works as a "black-box" with your simulation code(s):
    - Data transferred via file read/write operations
    - Works on LINUX/UNIX, Mac OS, Windows
  - In use at SNL, LLNL, LANL, ORNL, Navy, NASA, Lockheed-Martin, 3M, Kodak, Goodyear, etc. and at numerous universities
  - Freely available worldwide via GNU General Public License
    - ~3000 downloads, approx several hundred "serious" users
  - DAKOTA team receives significant return on investment from external users:
    - Bug reports, compilations on new computer systems, suggestions for future R&D, research collaborations
  - DAKOTA enables sensitivity analysis, optimization, and uncertainty quantification w/ high-fidelity simulation tools on massively-parallel supercomputers.

**roughly 500k lines of code total, with ~100k in DAKOTA "core"*

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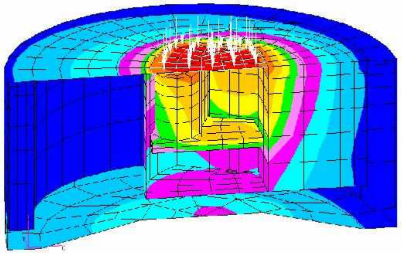
What is the Role of DAKOTA in Engineering/Science Applications?

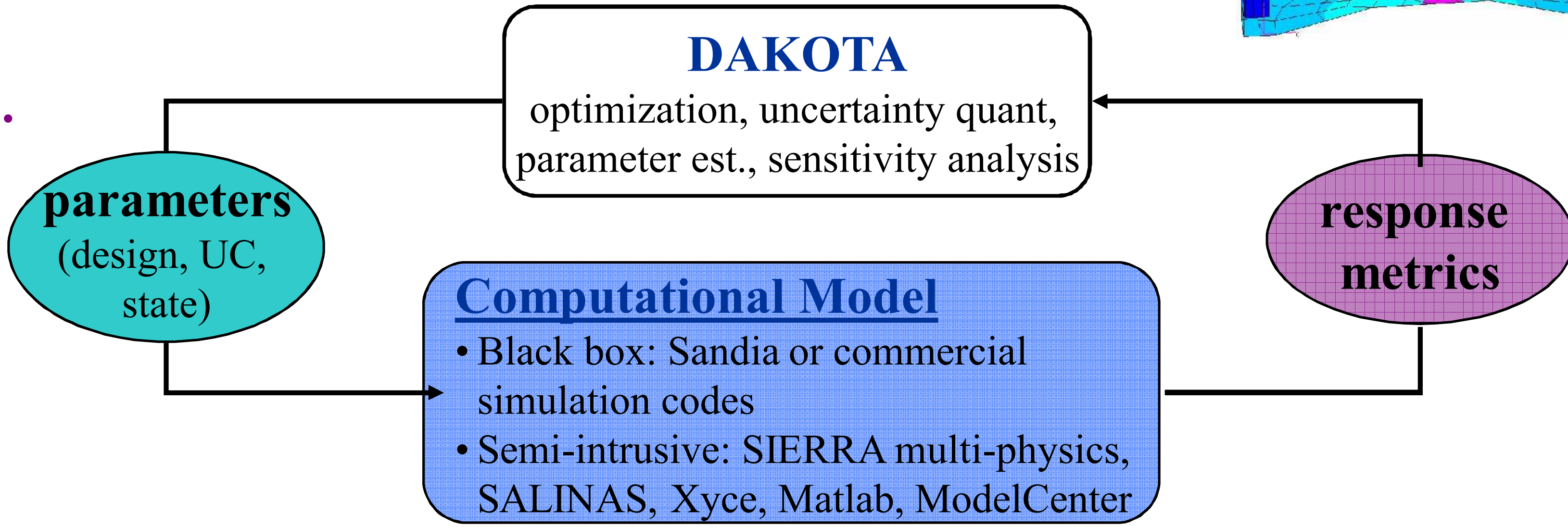
- **DAKOTA enables sensitivity analysis, optimization, and uncertainty quantification (UQ) to help answer "what if..." questions.**
  - What happens to my cost (or safety margin or performance level or ...) if I change parameter X?"
  - How reliable is my design?
  - How safe is my design?
  - What is the best design?

- **DAKOTA assists the analyst/designer in understanding and managing complex computer models.**
  - Automate typical "parameter variation" studies.
  - Discover/predict nonlinear interactions among many parameters.
    - Interactions that might be missed with traditional "change one parameter at a time" studies.
  - Support experimental testing efforts:
    - Examine many accident conditions with computer models, then physically test only a few of the worst-case conditions.

DAKOTA Overview



iterative analysis…

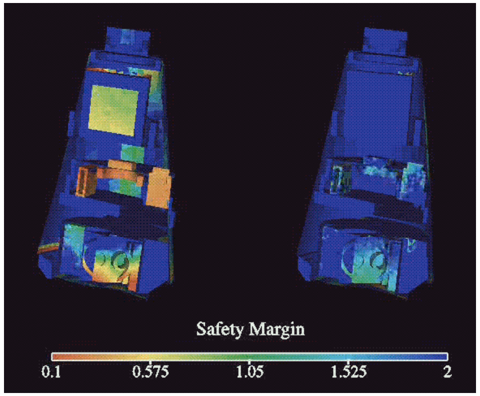


Goal: answer fundamental engineering questions

- 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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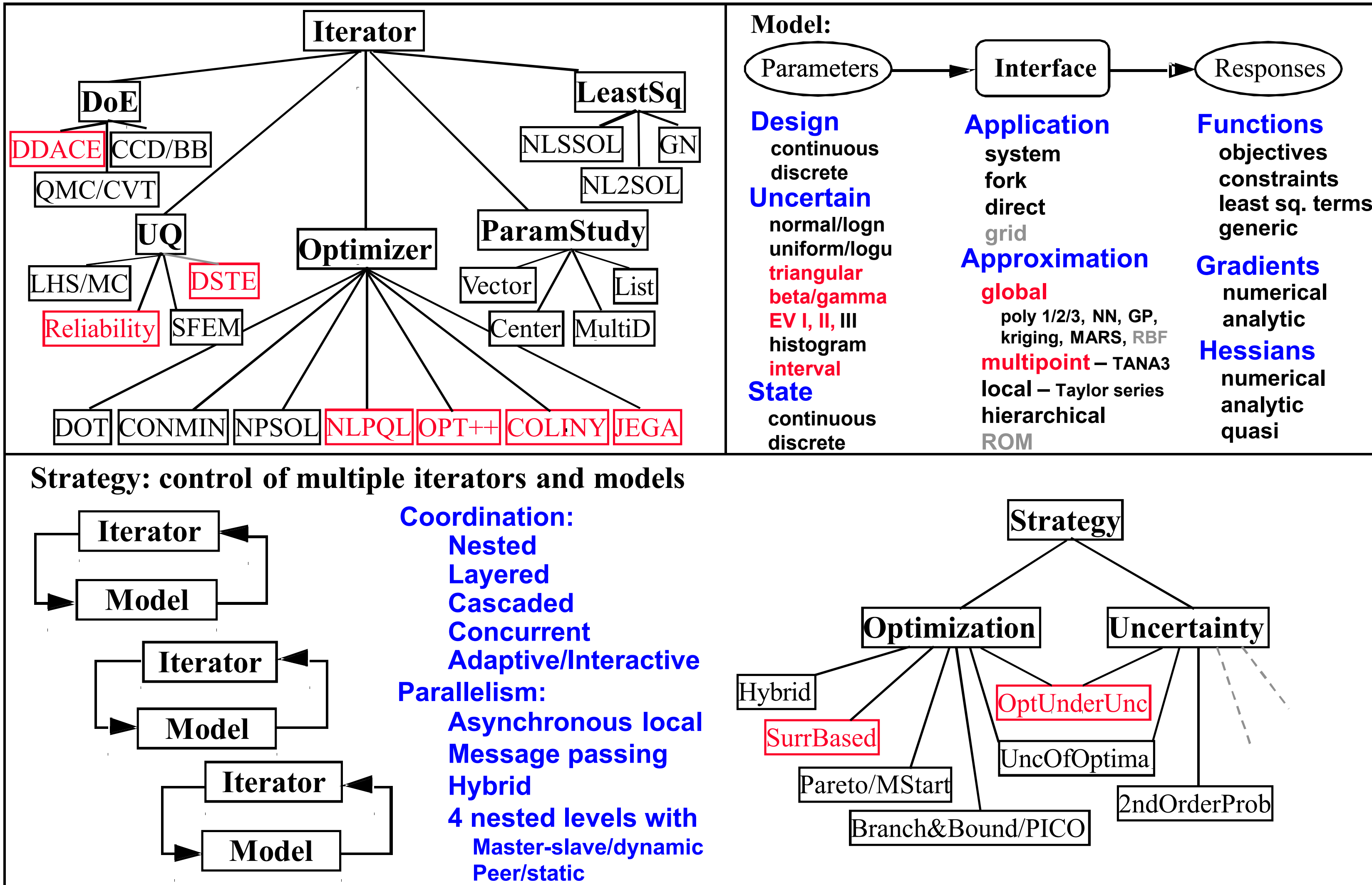
DAKOTA Framework



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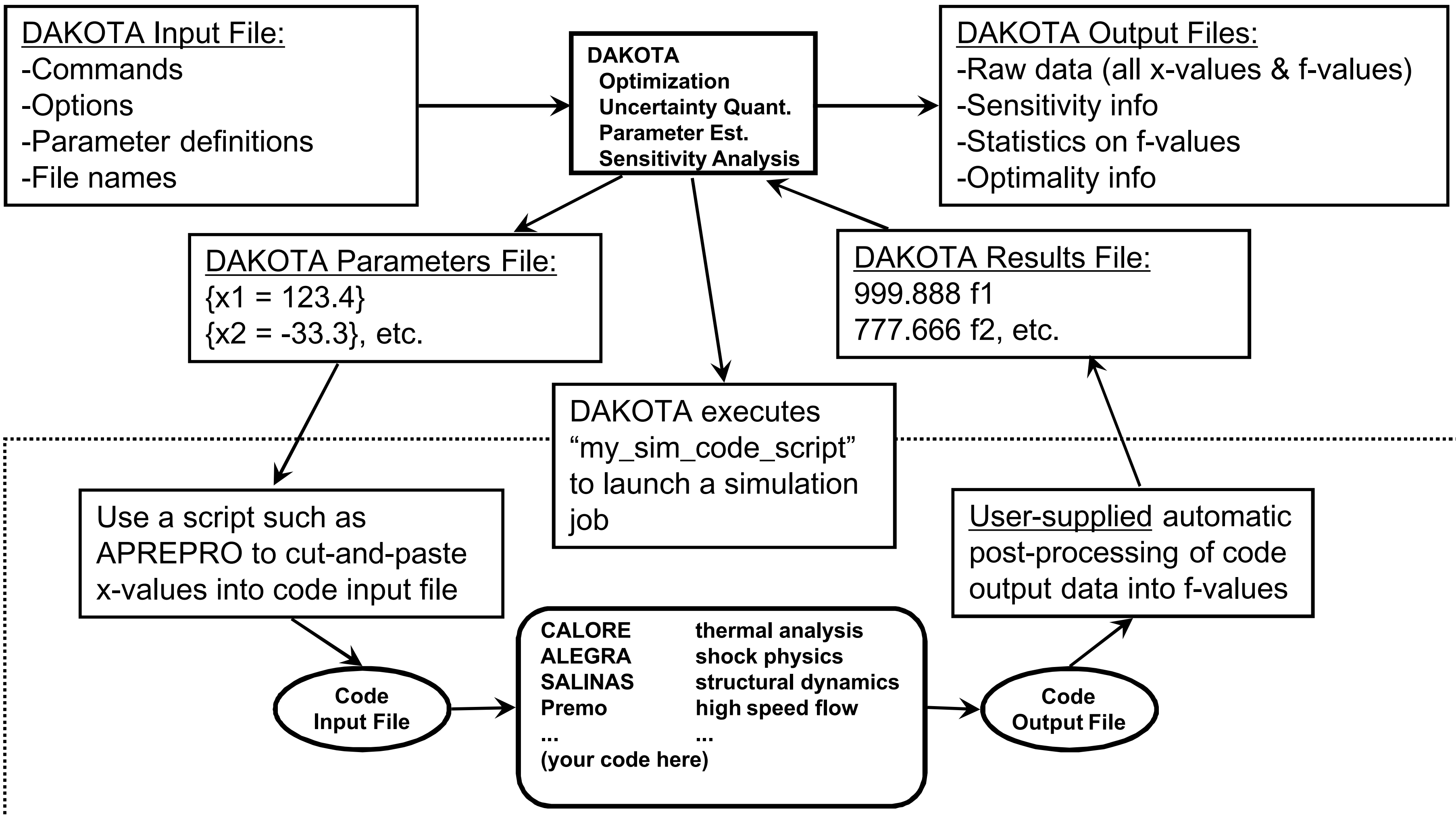
DAKOTA Execution & Info Flow

- What files go into DAKOTA?
- What files come out of DAKOTA?
- How does DAKOTA interact with my simulation code?

DAKOTA Execution & Info Flow



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Questions to Consider Before Using DAKOTA

1. What do I want to find out?
   – Sensitivity study? Optimization study? UQ study?

2. How many runs of my simulation code can I afford?
   – 10’s, 100’s, 1000’s, more?
   – How many processors per simulation code run?

3. Where am I going to run the simulation code?
   – On my PC? On my Mac?
   – On my Linux/Sun/SGI/IBM workstation?
   – On a network of workstations?
   – On a Linux/Sun/SGI/IBM cluster?
   – On a special supercomputer?

Of these, #1 and #2 are the most critical!

Overview: Model-based Uncertainty Quantification

Forward propagation: quantify the effect that uncertain (nondeterministic) input variables have on model output

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

(possibly given distributions)

Potential Goals:

- **based on uncertain inputs (UQ), determine variance of outputs and probabilities of failure (reliability metrics)**
- **identify parameter correlations/local sensitivities, robust optima**
- **identify inputs whose variances contribute most to output variance (global sensitivity analysis)**
- **quantify uncertainty when using calibrated model to *predict***

Methods:

- **Aleatoric/irreducible: sampling (Monte Carlo, LHS, CVT), reliability analysis (mean value, FORM, algorithmic variants)**
- **Epistemic/reducible: 2nd order probability, Dempster-Shafer Theory of Evidence**

DACE Methods

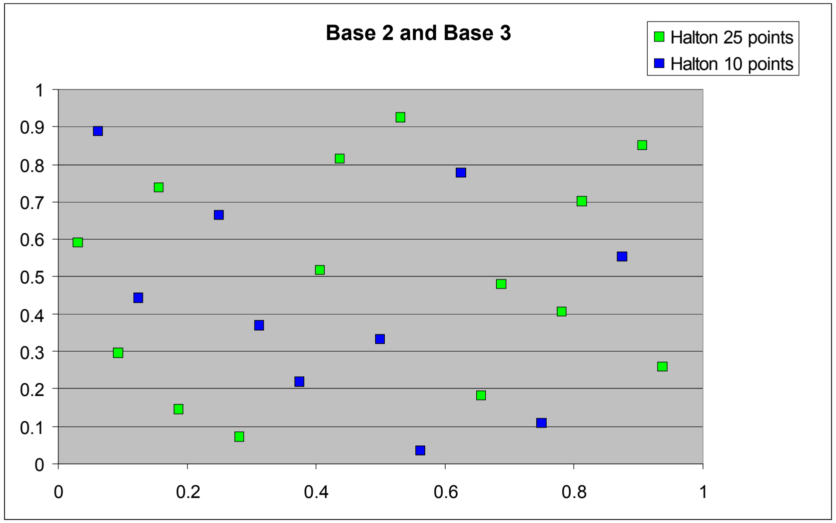
- Design of Computer Experiments
  - Usually, we do not assume distributional forms for the inputs
  - DDACE – Developed at SNL-CA (Monica Martinez-Canales)
    - Orthogonal arrays
    - Central Composite
    - Box-Behnken
    - Grid sampling
    - LHS and pure MC
    - Orthogonal LHS
    - Can calculate main effects for OAs
    - Can use in Variance Based Decomposition, Quality Metrics
  - FSUDACE – Developed by Florida State University, Max Gunzburger and John Burkardt
    - Halton sequences
    - Hammersley sequences
    - Centroidal Voronoi tesselation
    - Can "Latinize" these methods
    - Can use in Variance Based Decomposition, Quality Metrics
    - Fair amount of control in terms of where you want to start the sequence, what prime bases are used, etc.

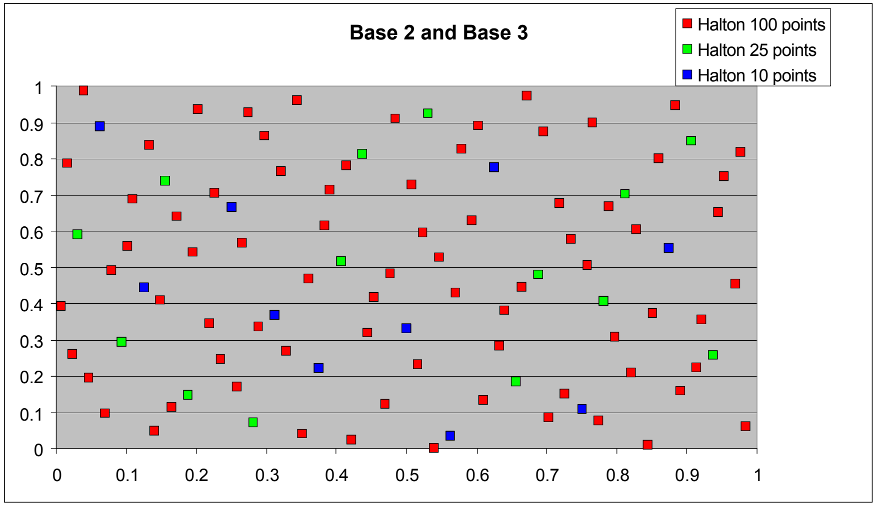
Quasi Monte Carlo Methods

- **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





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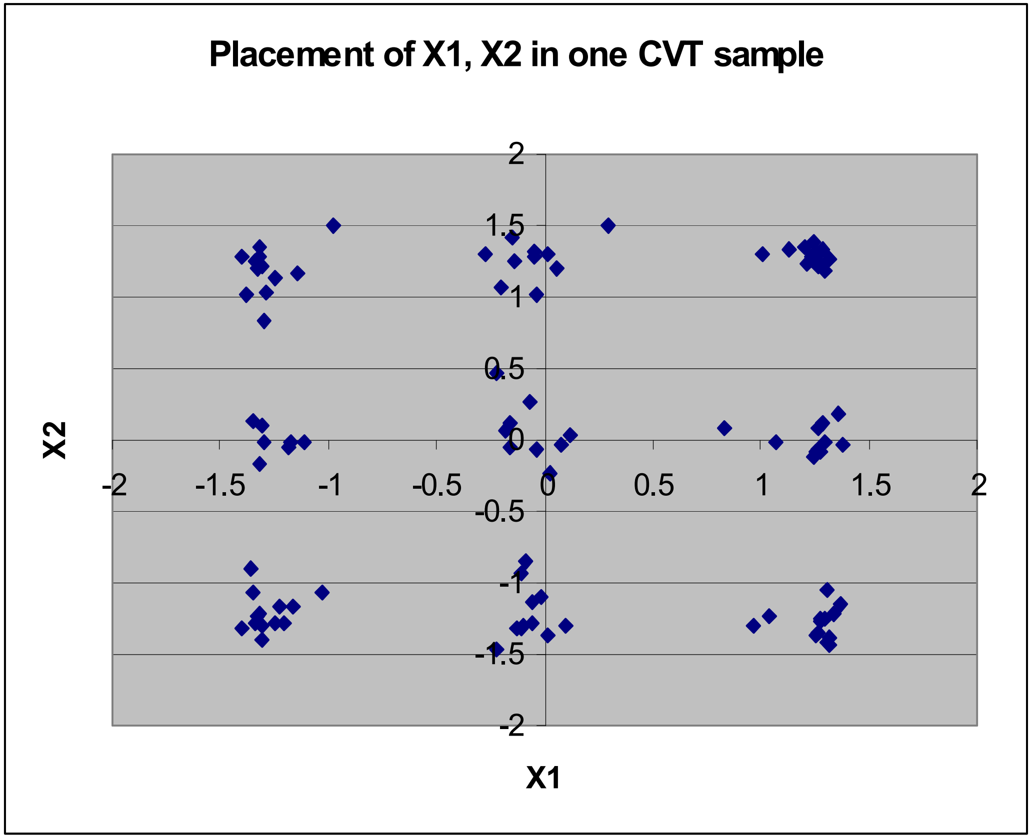
Quasi Monte Carlo Methods

- 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. Discrepancy is defined as the difference between the actual number and the expected number of points one would expect in a particular set B (such as a hyper-rectangle within the unit hypercube), maximized over all such sets.
- 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

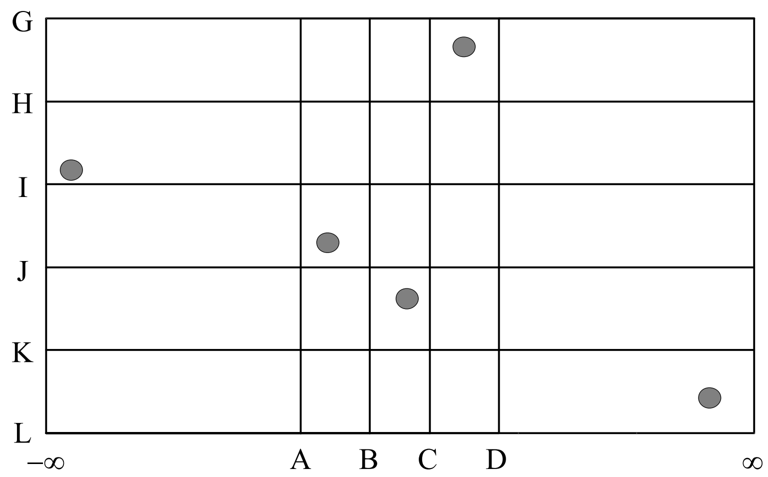


•This clustering may contribute to the method performing relatively well over all the space but poorly at the edges, which the RMSE metric emphasizes.

•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.

Sampling Methods

– **Latin Hypercube Sampling**
  - Distribution types supported: normal, lognormal, uniform, loguniform, triangular, gamma, gumbel, frechet, weibull, histogram, interval
  - Also can specify plain MC
  - Correlations between inputs supported with Iman and Conover's restricted pairing algorithm

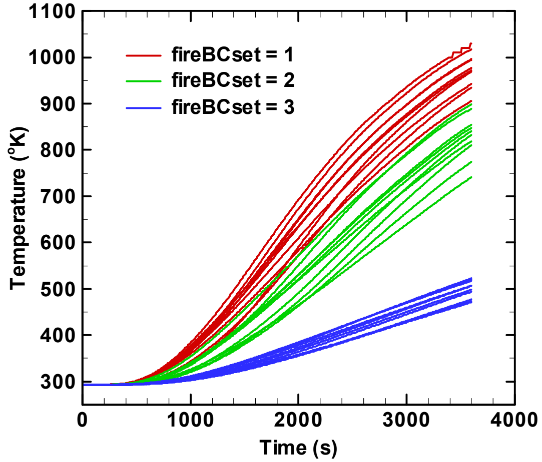


A Two-Dimensional Representation of One Possible LHS of size 5 Utilizing X1 (normal) and X2 (uniform)

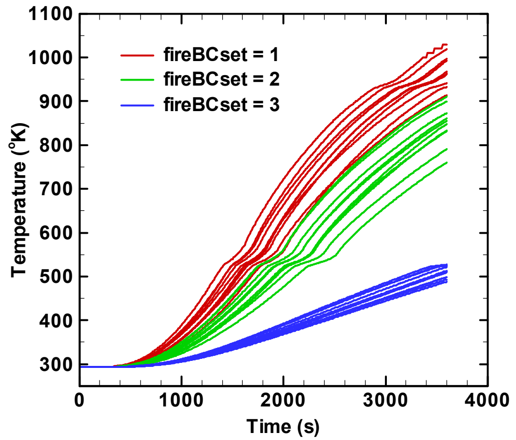
W76 Hydrocarbon Fire QMU Study
Component Temperature Responses

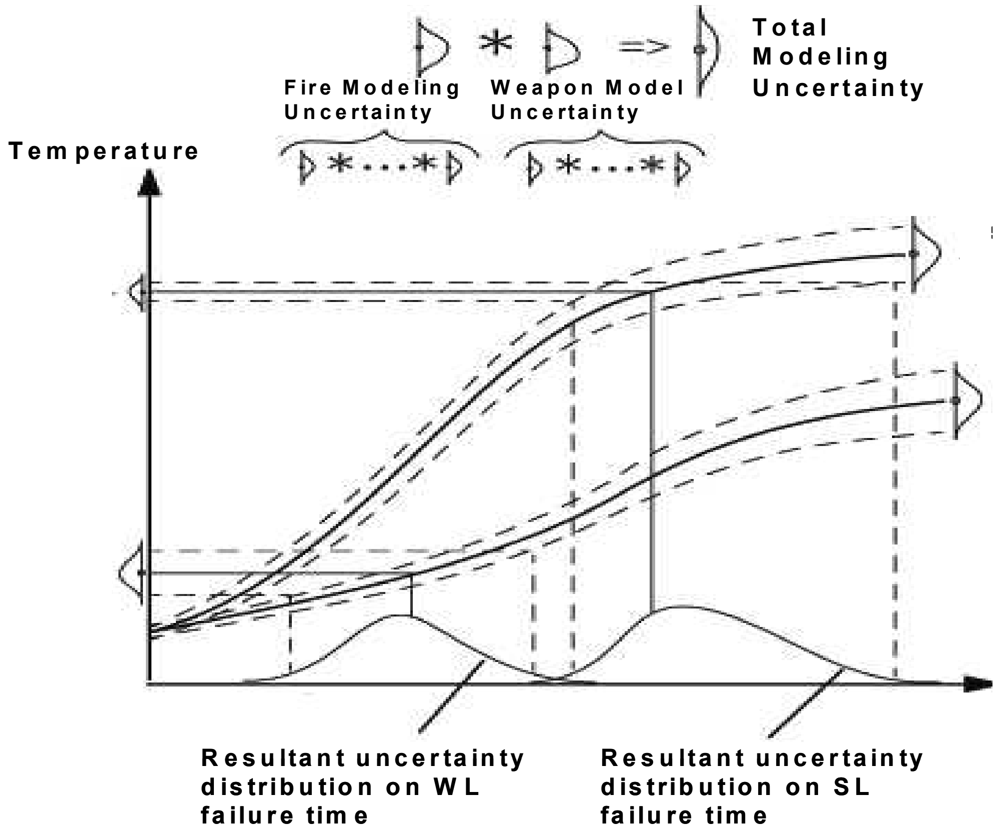
30 CALORE runs

Intent SL



Auxiliary capacitor WL





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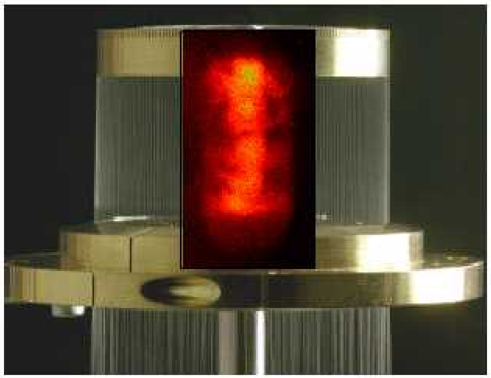
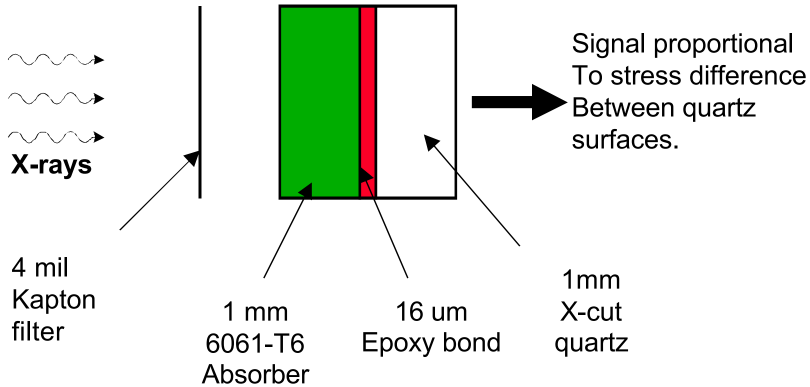
DAKOTA UQ Study: Presto Simulations vs. Z-Accelerator Data

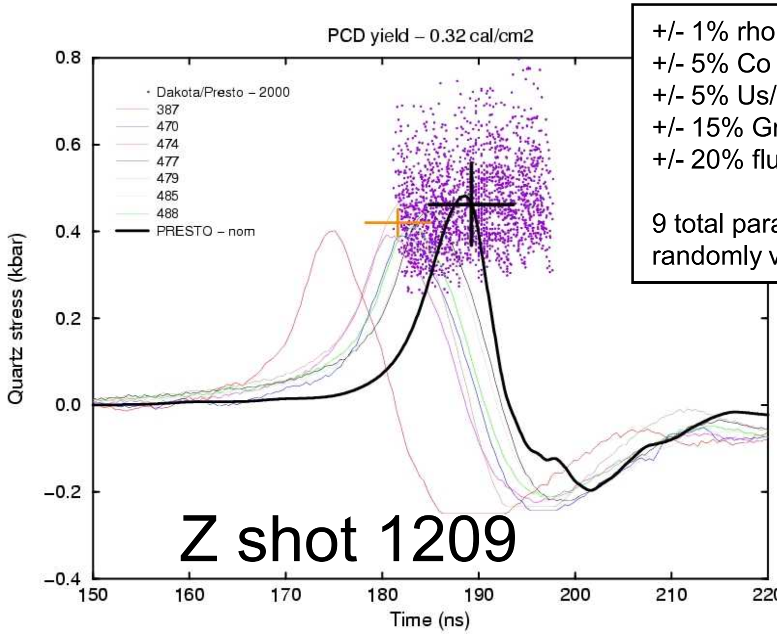
Tungsten wire array & Z pinch



X-Ray Induced Thermomechanical Shock Modeled w/ Presto

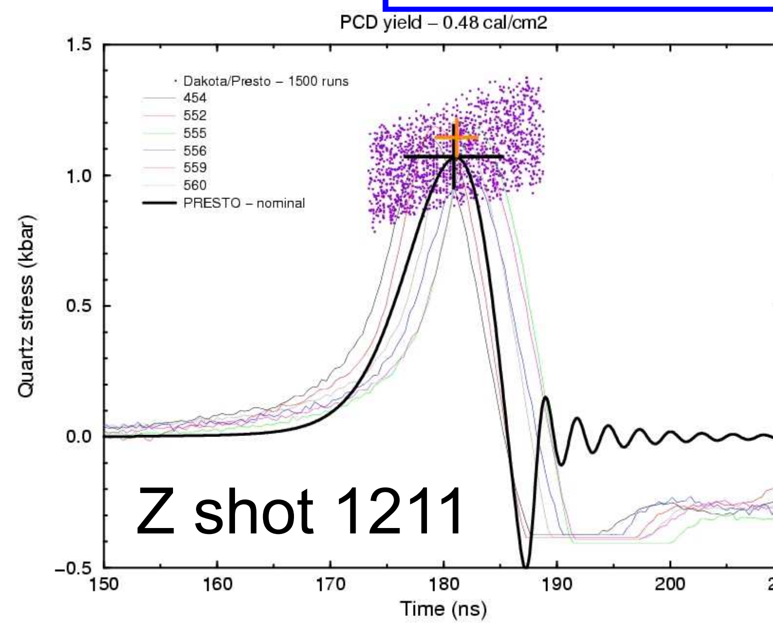


Summary:
- UQ study on Presto sims. of thermomechanical shock.
- DAKOTA generated 2000 Presto runs; run on 1500's network of workstations
- Compared Presto vs. Z Shot μ±1σ uncertainty bands.
- First-ever UQ study gives info on design margins. Need for Presto model improvement was identified.
- Contacts: Tony Giunta, 1533 & Joel Lash, 1514



+/- 1% rho
+/- 5% Co
+/- 5% Us/Up slope
+/- 15% Gruneisen
+/- 20% fluence

9 total parameters randomly varied



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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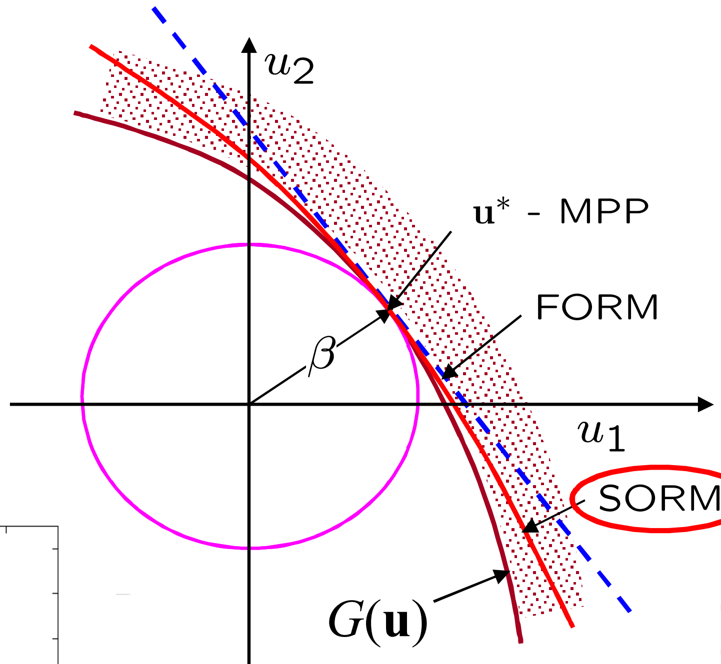
Analytic Reliability: MPP Search

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)

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

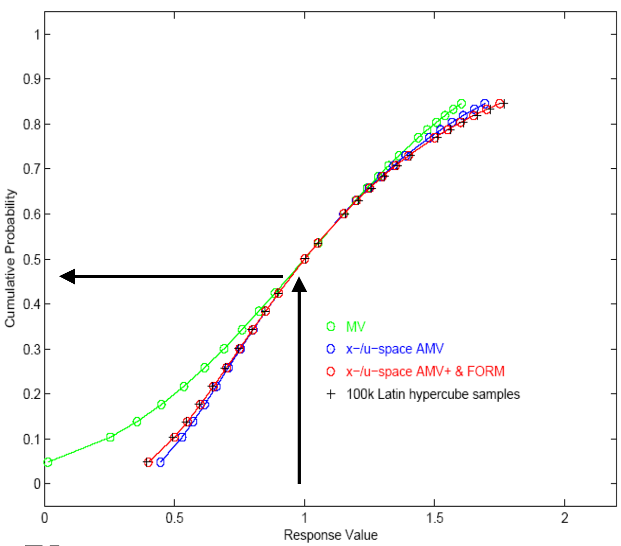
Find minimum distance to *G(u)* level curve; used for forward map *z* → *p or* β



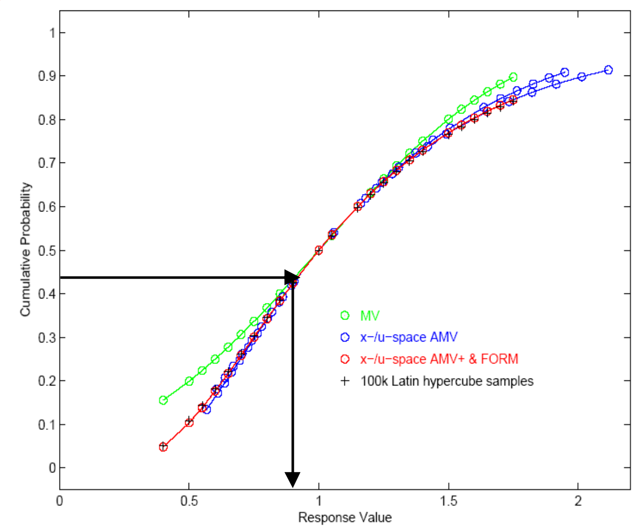
Performance Measure Approach (PMA)

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

Find minimum *G(u)* for specified β radius; used for inverse map *p* or β → *z*

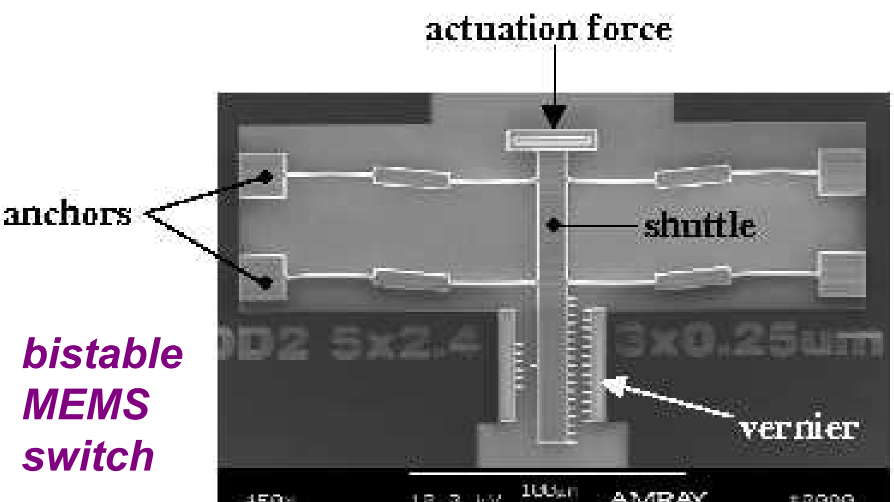


...should yield better estimates of reliability than Mean Value methods



Shape Optimization of Compliant MEMS

- Micro-electromechanical system (MEMS) made from silicon, polymers, and metals; used as micro-scale sensors, actuators, switches, and machines
- MEMS designs are subject to substantial variabilities and lack historical knowledge base
- Micromachining, photo lithography, etching processes yield uncertainty:
  - Material properties, manufactured geometries, residual and yield stresses
  - Material elasticity and geometry key for bistability
  - Data can be obtained to inform probabilistic approaches
- Resulting part yields can be low or have poor cycle durability
- Goal: shape optimization for bistable switch to…
  - Achieve prescribed reliability in actuation force
  - Minimize sensitivity to uncertainties (robustness)



bistable MEMS switch

uncertainties to be considered (edge bias and residual stress)

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

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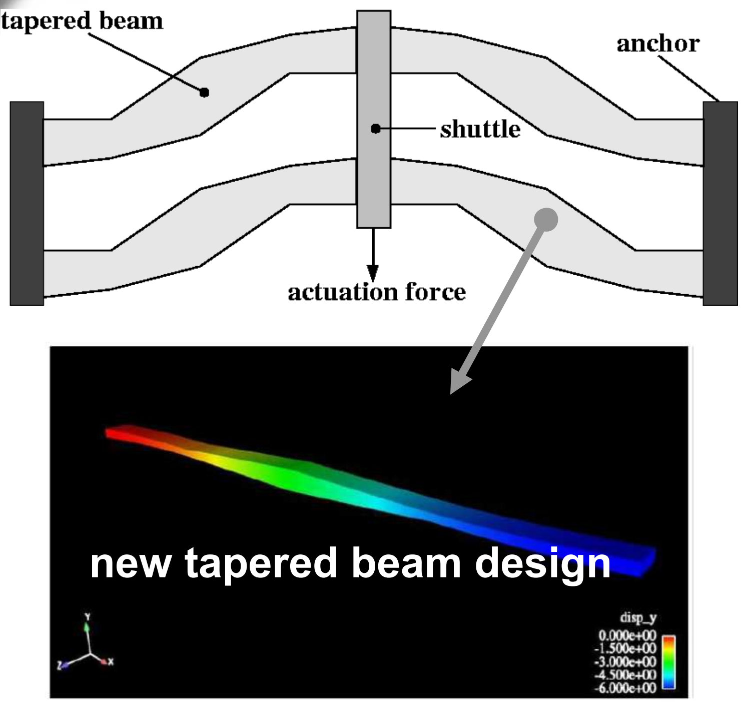
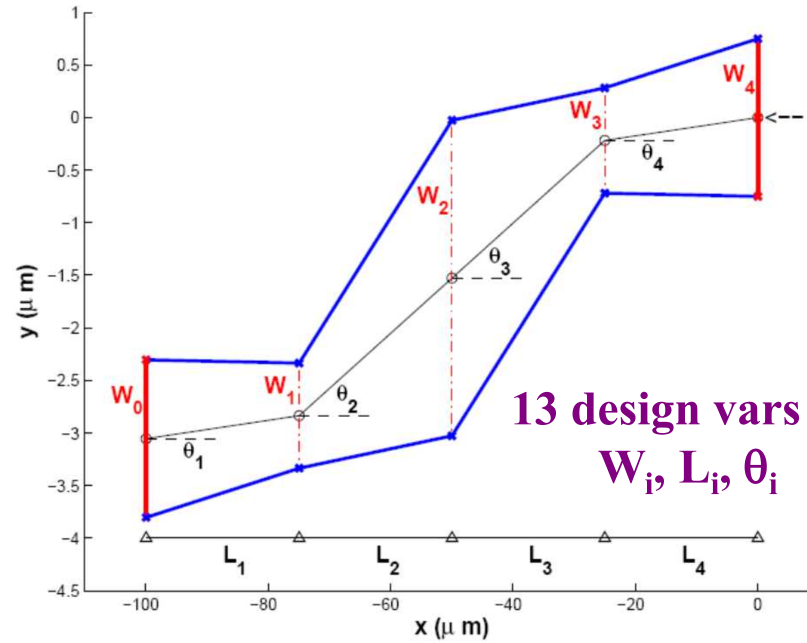
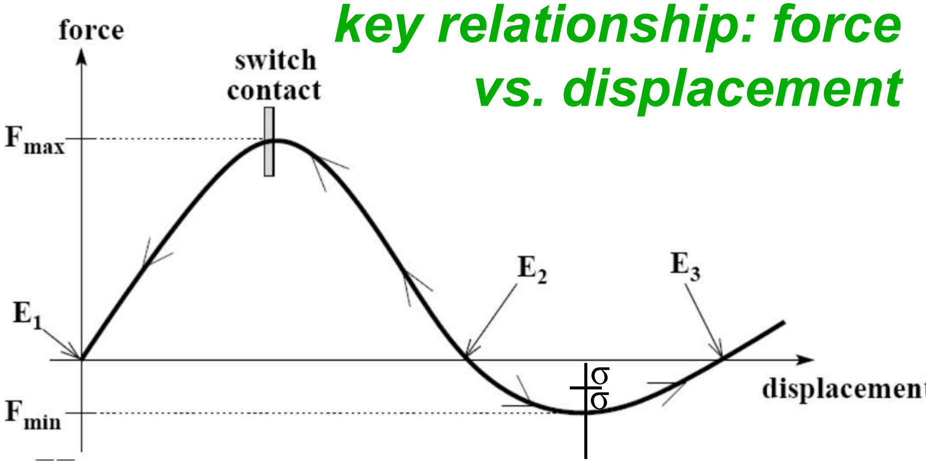
Tapered Beam Bistable Switch: Performance Metrics





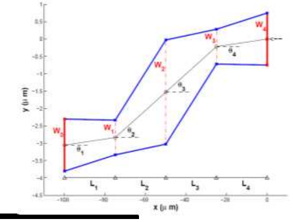
13 design vars *d*: W_i, L_i, θ_i

key relationship: force vs. displacement



Typical design specifications:

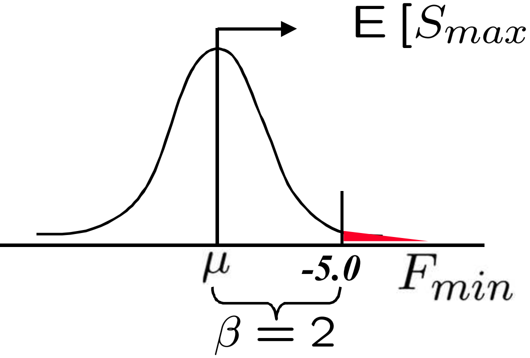
- **actuation force F_{min} reliably 5 μN**
- **bistable ($F_{max} > 0$, $F_{min} < 0$)**
- **maximum force: $50 < F_{max} < 150$**
- **equilibrium E2 < 8 μm**
- **maximum stress < 1200 MPa**

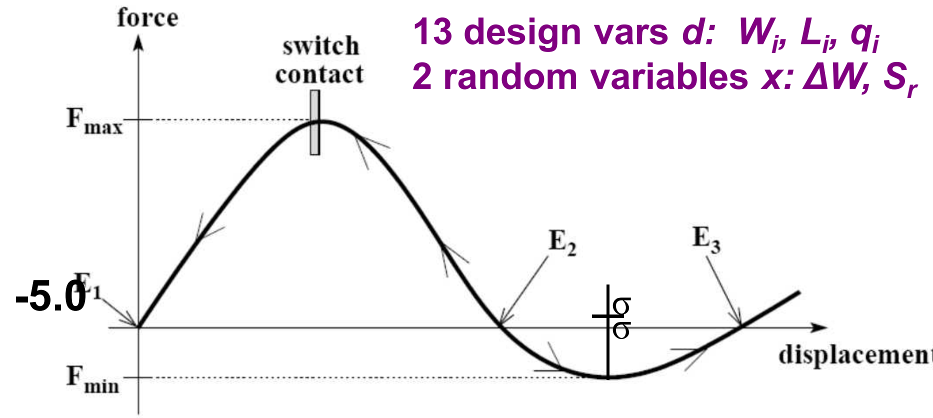


Bistable Switch: Problem Formulation

simultaneously reliable and robust designs

$$
\begin{array}{llll}
\max & & \mathrm{E}\left[F_{min}(\mathbf{d},\mathbf{x})\right] & \\
\text{s.t.} & 2 \leq & \beta_{ccdf}(\mathbf{d}) & \\
& 50 \leq & \mathrm{E}\left[F_{max}(\mathbf{d},\mathbf{x})\right] & \leq 150 \\
& & \mathrm{E}\left[E_2(\mathbf{d},\mathbf{x})\right] & \leq 8 \\
& & \mathrm{E}\left[S_{max}(\mathbf{d},\mathbf{x})\right] & \leq 3000
\end{array}
$$

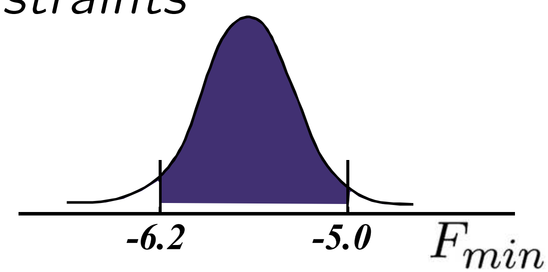




13 design vars *d*: W_i, L_i, q_i
2 random variables *x*: ΔW, S_r

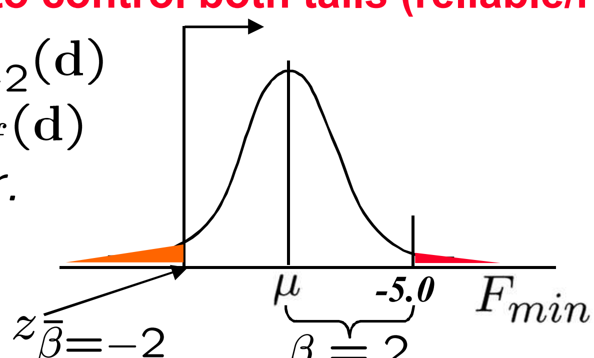
probability formulation – robust designs:

$$
\begin{array}{ll}
\max & \mathrm{P}\left(-6.2 \leq F_{min}(\mathbf{d}) \leq -5.0\right) \\
\text{s.t.} & \textit{nonlinear constraints}
\end{array}
$$



combined RIA/PMA to control both tails (reliable/robust):

$$
\begin{array}{lll}
\max & & z_{\bar{\beta}=-2}(\mathbf{d}) \\
\text{s.t.} & 2 \leq & \beta_{ccdf}(\mathbf{d}) \\
& & \textit{nln. constr.}
\end{array}
$$



(DAKOTA flexibly allows RIA/PMA combinations)

Reliability Formulation Results

RBDO with Mean Value, AMV2+, and FORM for reliability analysis

variable/metric				MVFOSM	AMV^2+	FORM
l.b.	name	u.b.	initial $\mathbf{d}^0$	optimal $\mathbf{d}^*_M$	optimal $\mathbf{d}^*_A$	optimal $\mathbf{d}^*_F$
10	$L_1\,(\mu m)$	35	25.0	19.23	28.04	28.06
10	$L_2\,(\mu m)$	35	25.0	28.44	24.42	24.45
10	$L_3\,(\mu m)$	35	25.0	14.44	30.58	30.68
10	$L_4\,(\mu m)$	35	25.0	35.00	30.55	30.66
0	θ_1 (deg.)	5	1.0	2.733	4.200	4.189
0	θ_2 (deg.)	5	3.0	2.260	2.481	2.488
0	θ_3 (deg.)	5	3.0	2.719	2.465	2.478
0	θ_4 (deg.)	5	1.0	3.230	2.384	2.390
1	$W_0\,(\mu m)$	3	1.7	1.058	1.355	1.346
1	$W_1\,(\mu m)$	3	1.2	2.038	1.275	1.265
2	$W_2\,(\mu m)$	5	3.2	2.390	3.481	3.488
1	$W_3\,(\mu m)$	3	1.2	1.312	2.006	2.004
1	$W_4\,(\mu m)$	3	1.7	1.000	1.333	1.333
	E $[F_{min}]$ (μN)		-26.29	-5.896	-6.188	-6.292
2	β		5.376	2.000	1.998	1.999
50	E $[F_{max}]$ (μN)	150	68.69	50.01	57.67	57.33
	E $[E_2]$ (μm)	8	4.010	5.804	5.990	6.008
	E $[S_{max}]$ (MPa)	1200	470	1563	1333	1329
	AMV^2+ verified β		3.771	1.804	-	-
	FORM verified β		3.771	1.707	1.784	-

- significant improvement in minimum force
- β constraint active at optimal designs

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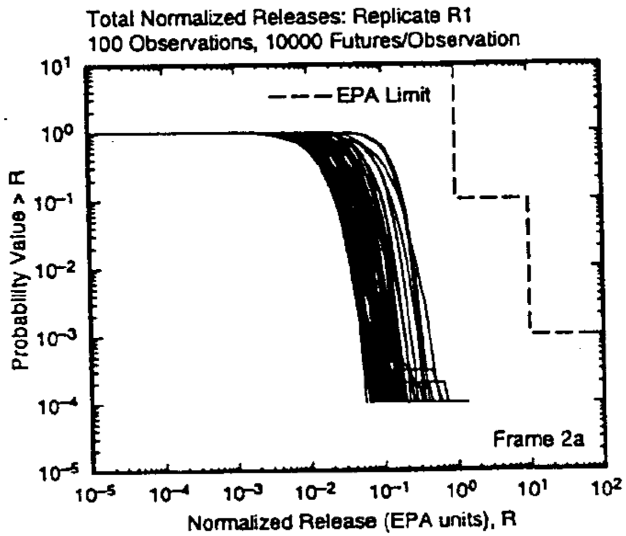
Epistemic UQ

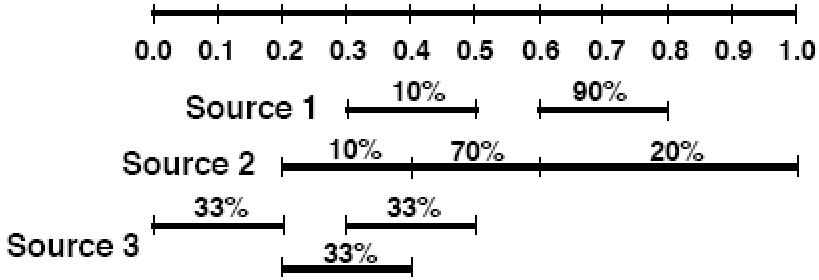
Second-order probability

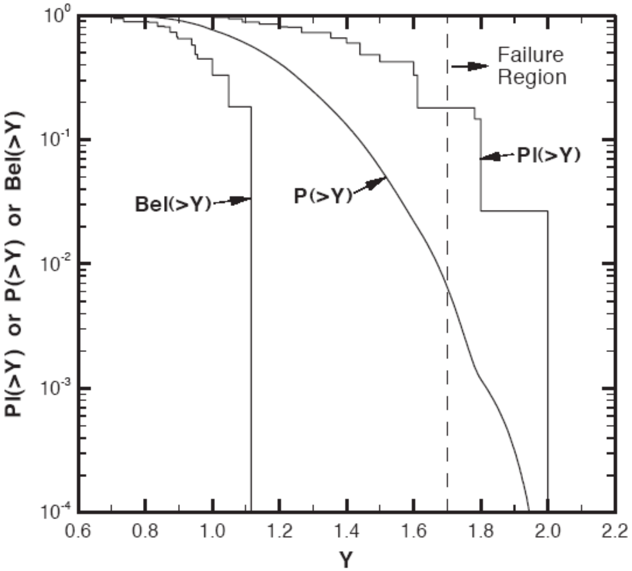
- Two levels: distributions/intervals on distribution parameters
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).



Dempster-Shafer theory of evidence

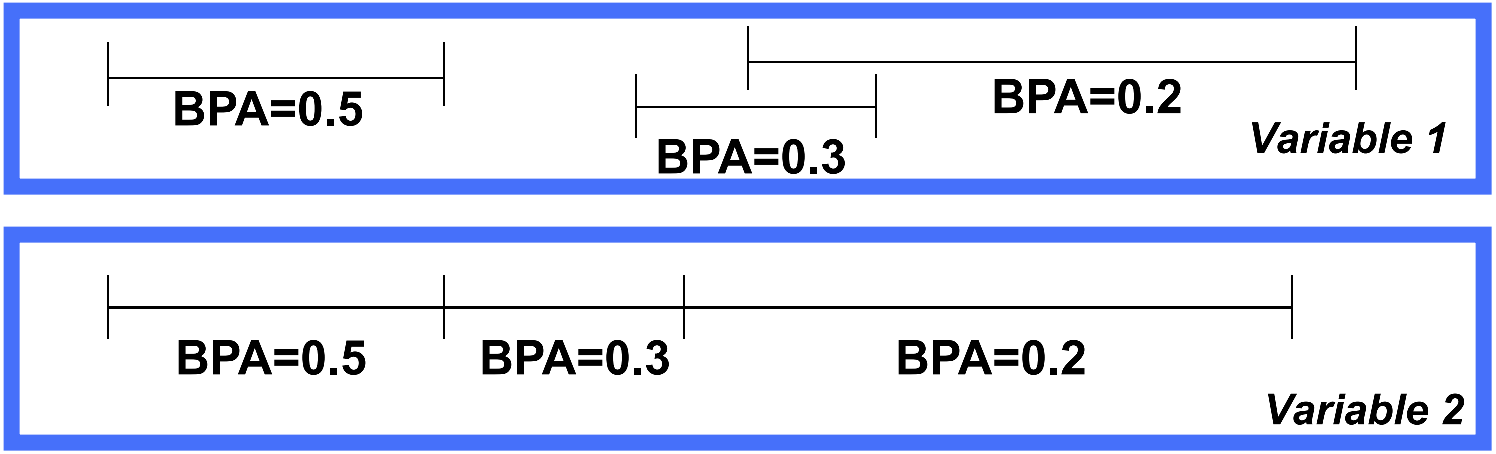
- Basic probability assignment (interval-based)
- Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals





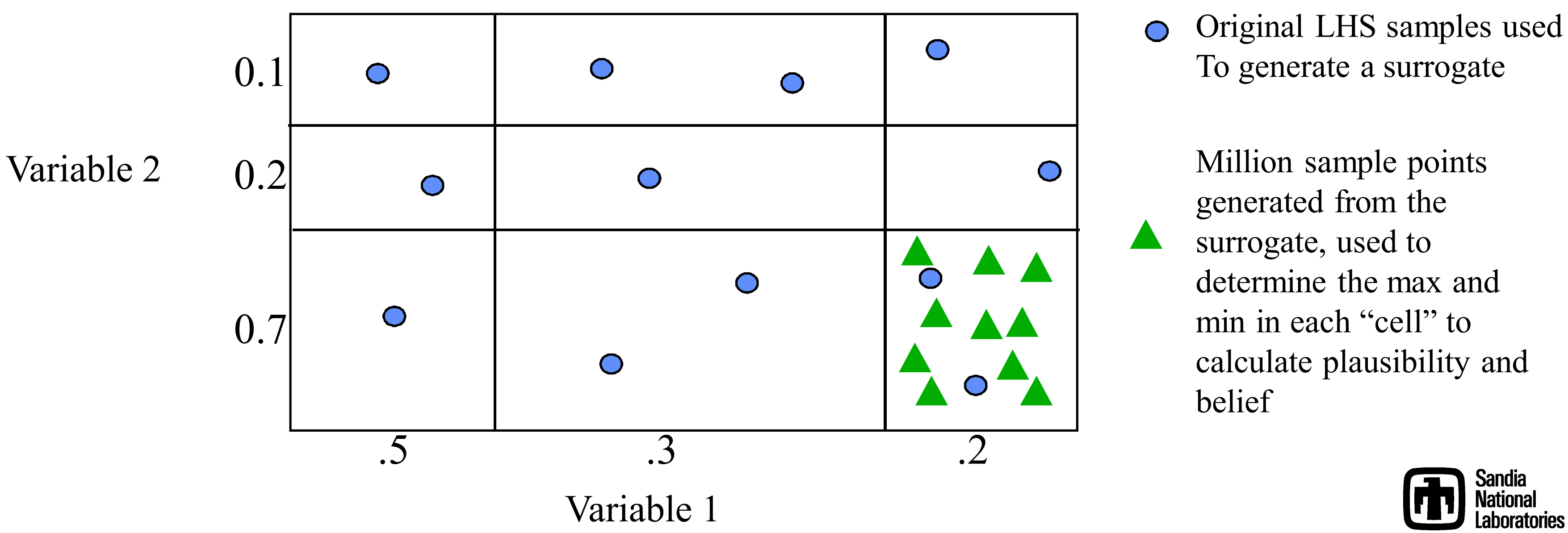
Epistemic Uncertainty Quantification

- 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
- The implication is that if you had more time and resources to gather more information, you could reduce the 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”

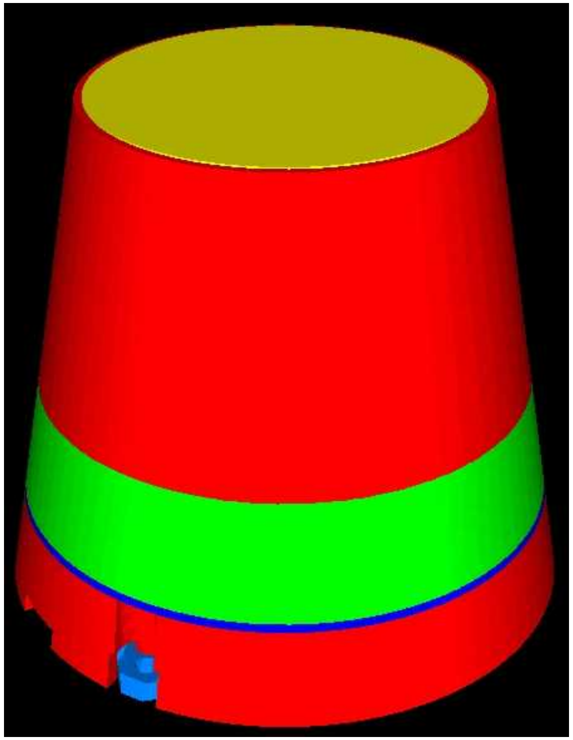


Epistemic Uncertainty Quantification

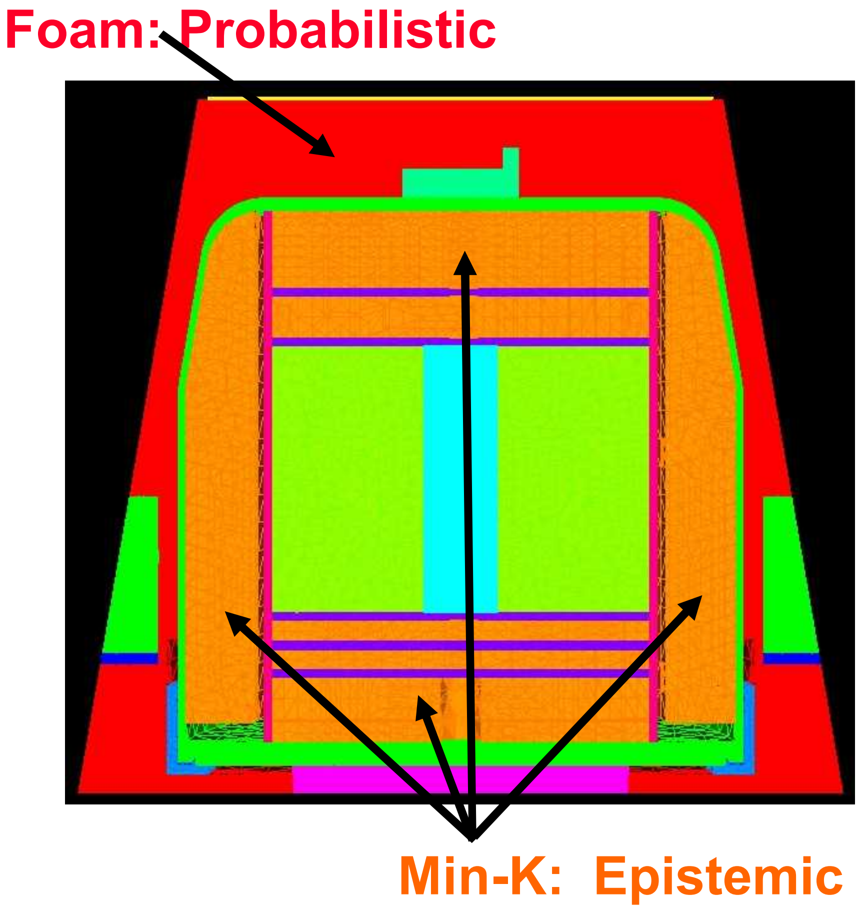
- **Look at various combinations of intervals. In each joint interval "box", one needs to find the maximum and minimum value in that box (by sampling or optimization)**
- **Belief is a lower bound on the probability that is consistent with the evidence**
- **Plausibility is the upper bound on the probability that is consistent with the evidence**
- **Order these beliefs and plausibility to get CDFs**
- **Draws on the strengths of DAKOTA**
  - **Requires surrogates**
  - **Requires sampling and/or optimization for calculation of plausibility and belief within each interval "cell"**
  - **Easily parallelized**



ASC V&V Thermal Battery Assembly



Thermal Battery Assembly (TBA)

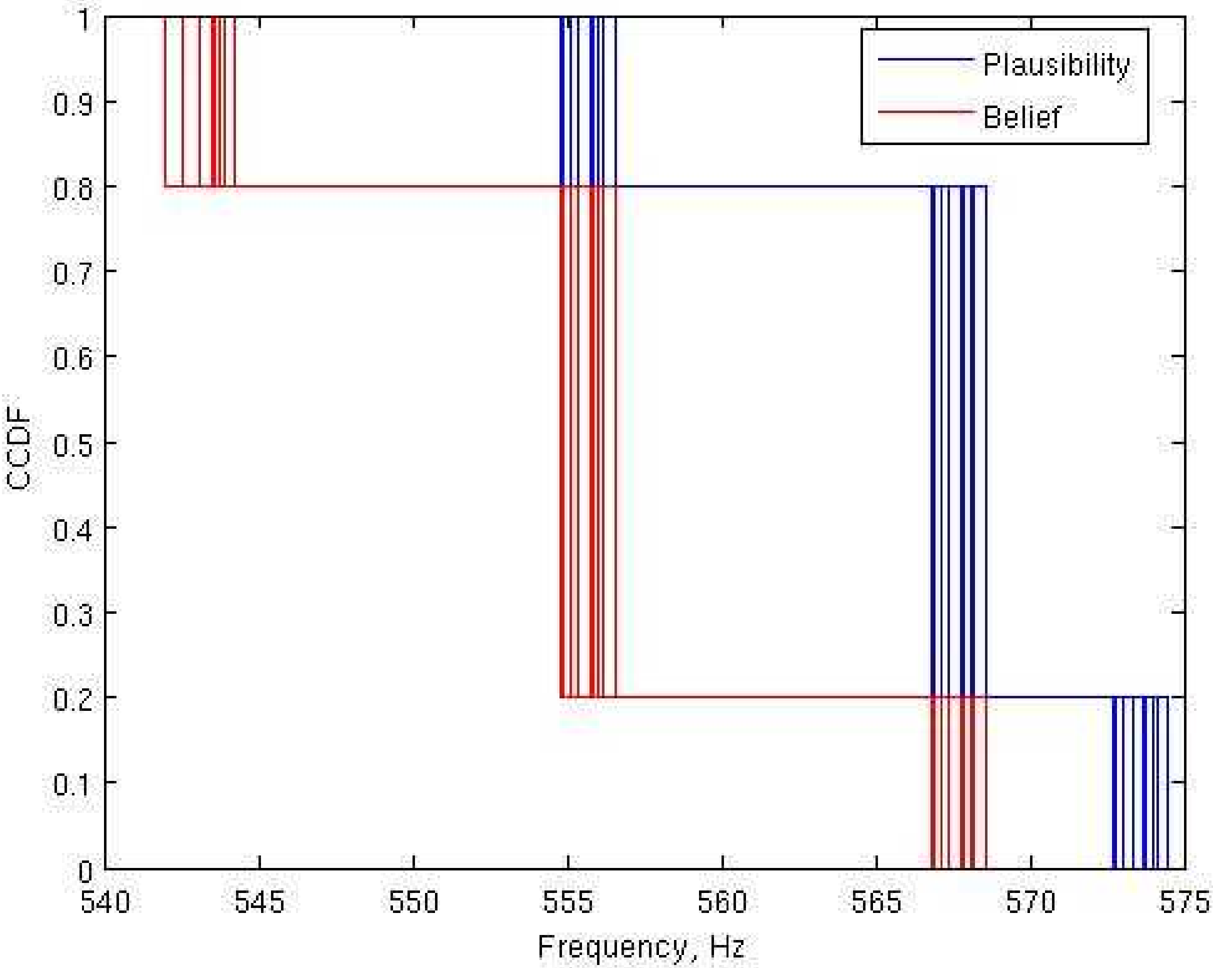


Thermal Battery Assembly Epistemic UQ

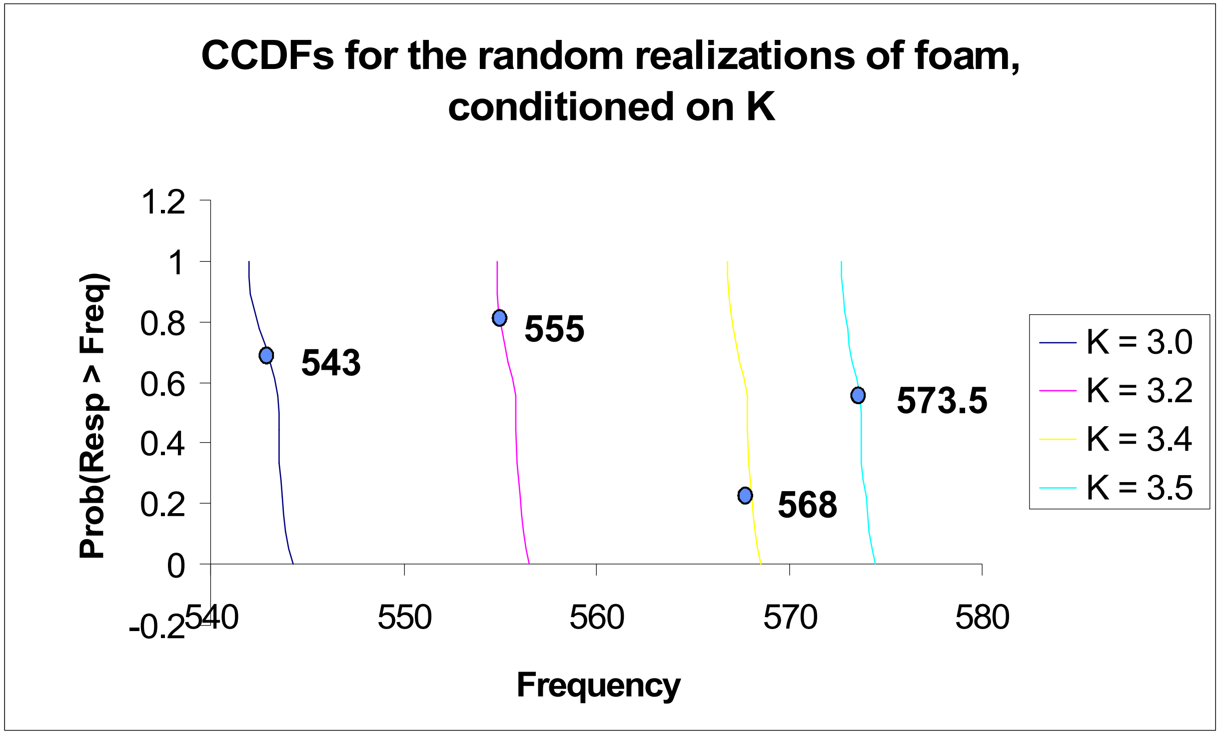
- **Treated the elastic property of min-K as an epistemic variable with 3 intervals: [3.0, 3.2] (3.2,3.4], and (3.4, 3.5]**
- **Treated the foam density as a probabilistic variable**

Min K	**Foam**
	**Probabilistic** • **Used a kernel density estimator based on actual data**

Thermal Battery Assembly CCDFs for Belief and Plausibility



Different Representation of the Epistemic Uncertainty



P(Freq > 555|K=3.2) = 1 if Freq < 554.8
0 if freq > 556.5
177.4 – 0.49F + 29.73 K

•Idea is to look at the range of the exceedence probability (CCDF value) given the epistemic structure on K

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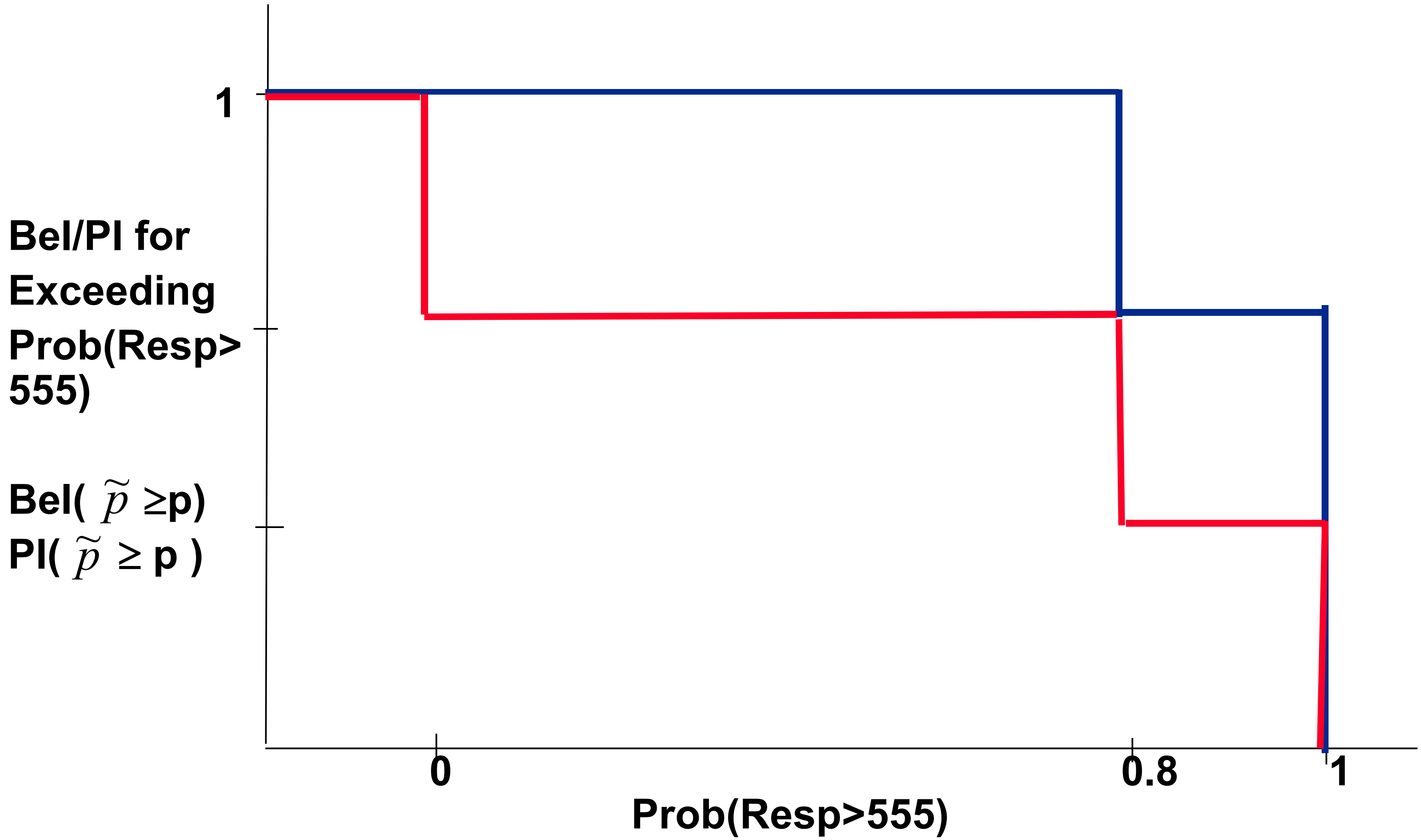
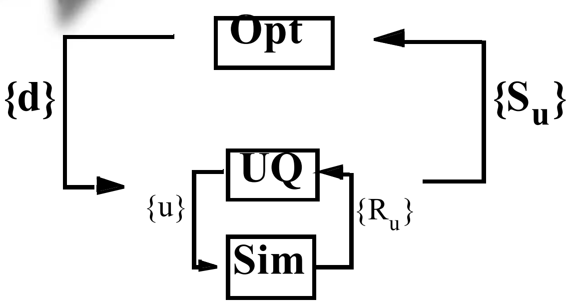
Calculation of Belief and Plaus for K=3.2, q=555



Optimization Under Uncertainty



nested paradigm

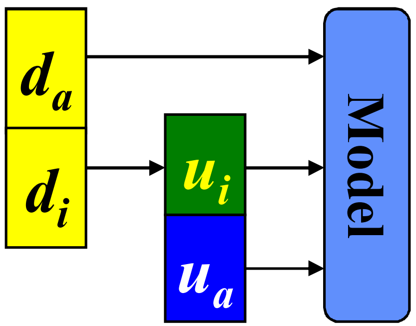
optimize, accounting for uncertainty metrics

(use any of UQ/reliability methods)

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

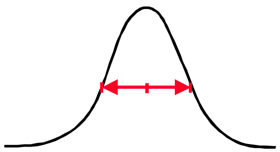
Input design parameterization

- Uncertain variables **augment** design variables in simulation
- **Inserted** design variables: an optimization design variable may be a parameter of an uncertain distribution, e.g., design the mean of a normal.

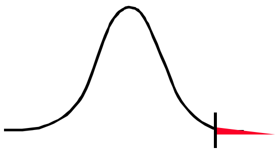


Response metrics to design for…

…robustness:
min/constrain μ, σ^2, moments or G(β) range



…reliability:
max/constrain *p*/β (minimize tail stats, failure)



…combined/other:
pareto tradeoff, LSQ: model calibration under uncertainty

Conclusions

- The DAKOTA toolkit includes algorithms for uncertainty quantification and optimization with large-scale computational models.
- DAKOTA strategies enable combination of algorithms, use of surrogates and warm-starting, and leveraging massive parallelism.
- Uncertainty-aware design optimization is helpful in design where robust and/or reliable designs are essential.
- DAKOTA provides capabilities to enable QMU studies (Quantification of Margins and Uncertainties)

DAKOTA Team Contact Info

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Parting Thoughts....

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