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Epistemic Uncertainty Quantification Tutorial

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Epistemic vs. Aleatory Uncertainty

- **EPISTEMIC**
  - Lack of knowledge about the appropriate value to use for a quantity
  - Subjective uncertainty
  - Reducible uncertainty: uncertainty can be reduced through increased understanding (research), or increased and more relevant data.
  - Epistemic quantities have a fixed value in an analysis, but we do not know that fixed value.
  - E.g. the elastic modulus for the material in a specific component is presumably fixed but unknown or poorly known.

- **ALEATORY**
  - Uncertainty characterized by inherent randomness
  - Cannot be reduced by further data
  - Variability
  - Irreducible
  - E.g. the height of individuals in a population
  - Usually modeled with probability distributions

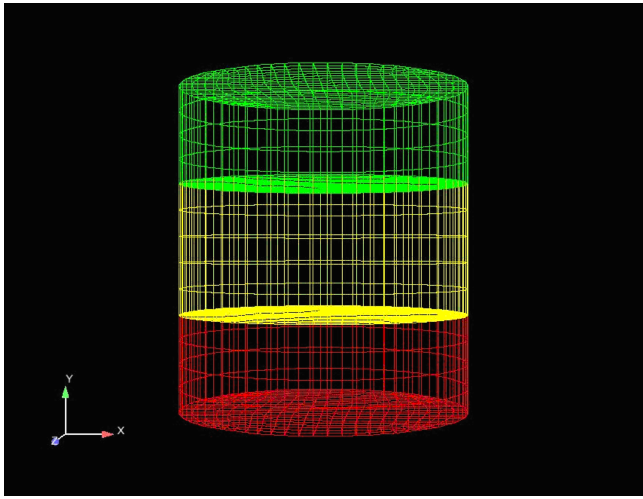
Engineering Applications Motivation

- Most computer models for engineering applications are developed to help assess a design or regulatory requirement.
- The capability to quantify the impact of uncertainty in the decision context is critical.
  - Example: Probability (System Response > T) < 0.01
- Still want to be able to provide bounds and other information when epistemic uncertainty exists
- This presentation discusses 3 methods for quantifying epistemic uncertainty
  - Interval Analysis
  - Dempster-Shafer theory of evidence
  - "Second-order" probability analysis
- These methods are all implemented in DAKOTA

Structural Dynamics Example

- 3-disc model for aeroshell.
- Outer 2 discs represent rigid masses
- Inner disc represents a layer of a filled rubber.

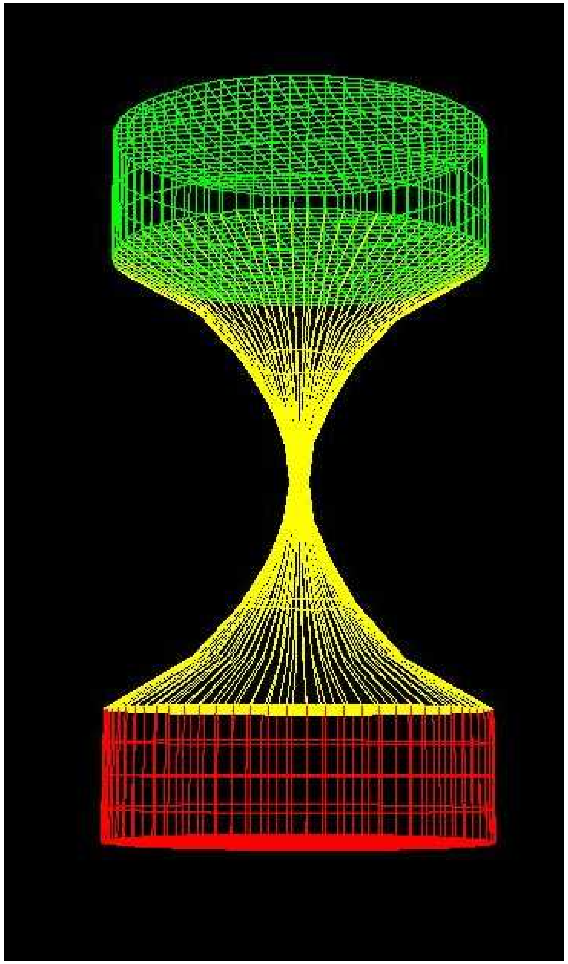
- We are interested understanding *the frequencies of the axial and shear modes for this experimental configuration.*
- There is significant epistemic uncertainty associated with the material properties of the filled rubber.
- We have a wide variety of tests and expert opinion on potential values for:
  - The modulus of elasticity. E falls within the interval of [2000, 25000] psi.
  - Poisson's ratio. ν falls within the interval of [0.45, 0.495].

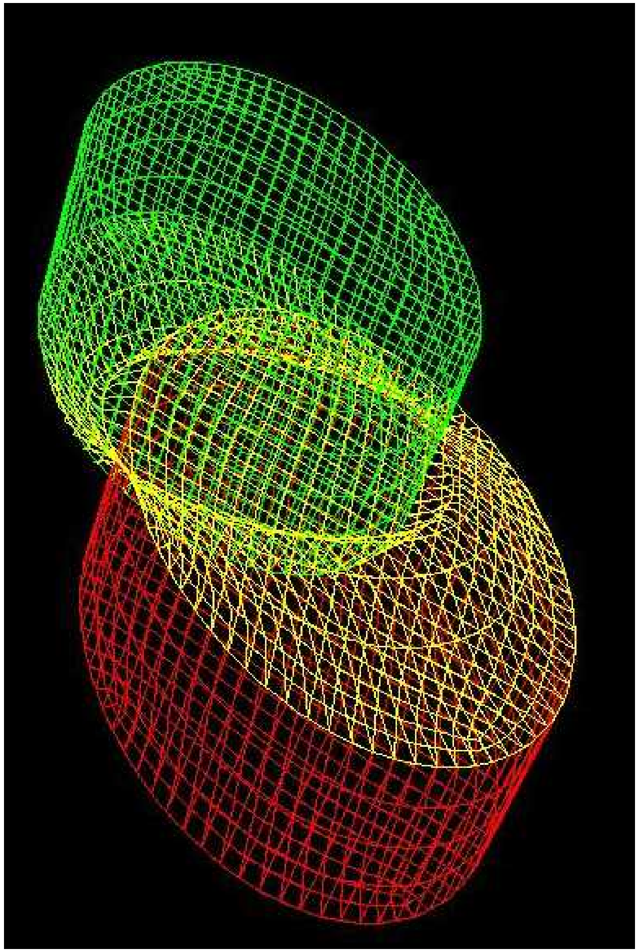


- The simulation code used is Salinas.
- The UQ code used is DAKOTA.

Structural Dynamics Example

- **What is the range of frequencies for the axial mode and the shear mode given the epistemic uncertainties in E and ν?**





Interval Analysis

- Specify intervals on uncertain inputs
- Determine the resulting interval on the output
- Example: A lies within the interval [3,5] and B lies within the interval [4,6]. The sum C = A + B is then contained within the interval [7,11].
- In practice, most realistic problems are not amenable to analytic calculations
- Options:
  - Sample from input intervals and obtain sample of output interval
  - Take initial samples over space, construct surrogate models, and query the surrogates extensively to understand upper and lower bounds on output
  - Use optimization methods

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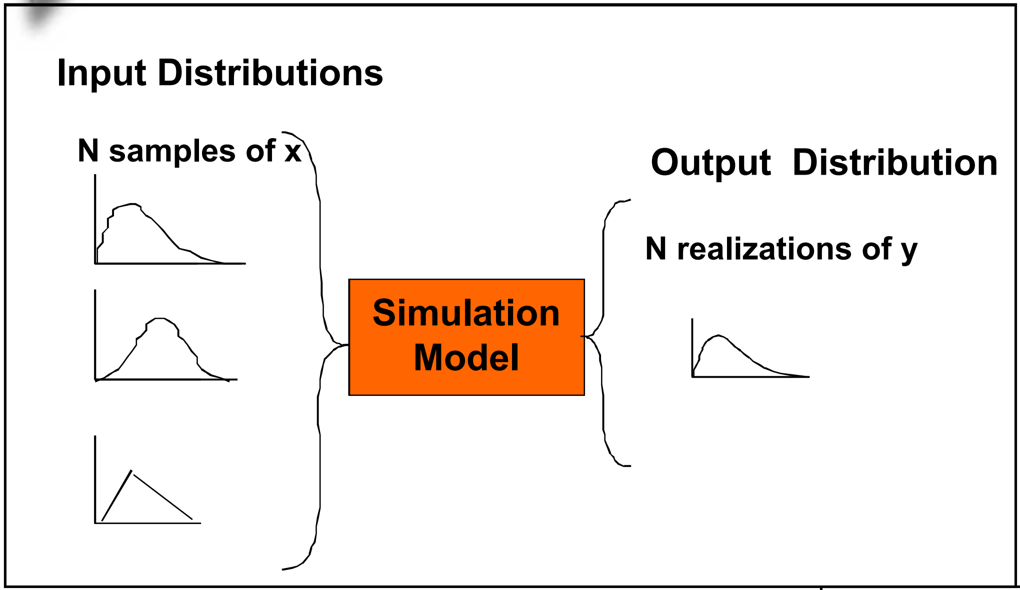
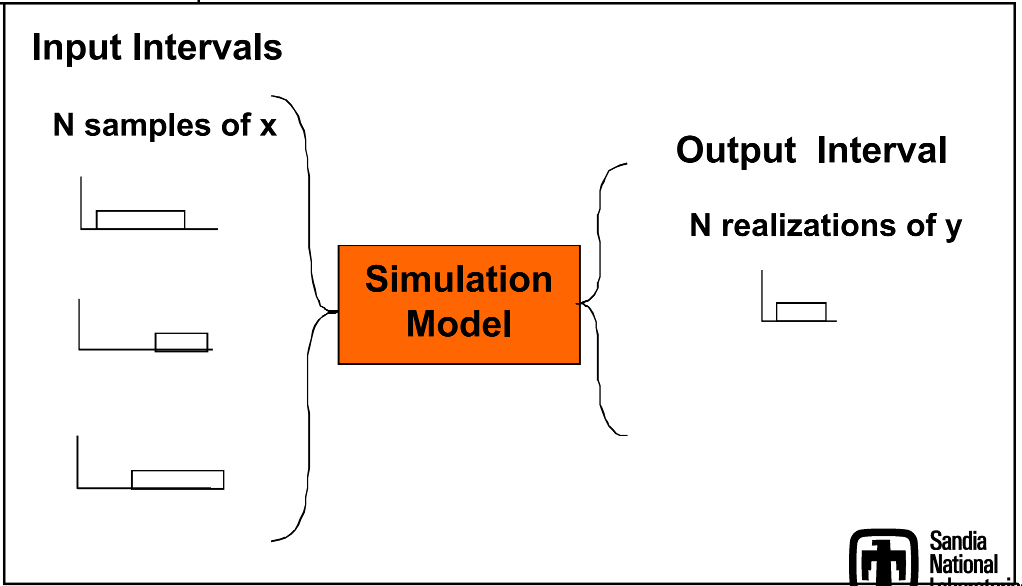
Interval Analysis: Sampling

Probabilistic



Non-Probabilistic



Caution: Do not put a frequency interpretation on the output when using sampling to determine intervals. Each output value is merely a possible or potential value, not a value from a distribution.

Interval Analysis: Sampling

Sample	E (Elastic Modulus)	Nu (Poisson's ratio)	Shear Mode Frequency	Axial Mode Frequency
1	6377.50	0.473	1452.47	1858.78
2	24938.67	0.455	2877.98	3580.37
3	9764.92	0.463	1799.41	2263.74
4	20550.80	0.462	2610.35	3277.82
5	14733.46	0.466	2209.13	2793.58
6	19525.95	0.488	2539.35	3333.59
7	12791.57	0.482	2055.63	2670.29
8	16942.52	0.481	2365.74	3065.20
9	7312.58	0.452	1559.74	1931.17
10	2162.54	0.476	845.62	1088.09

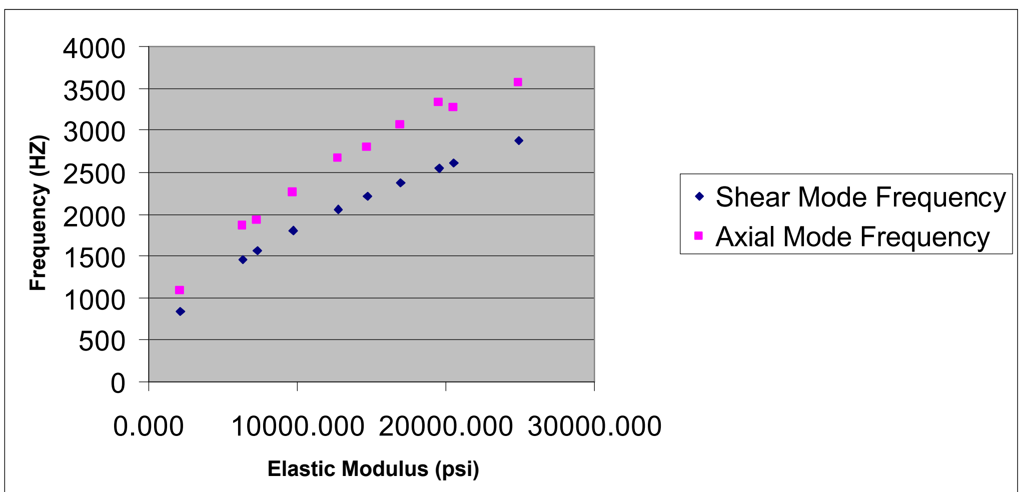
Shear mode frequency interval is: [845.6, 2878.0] Hz,

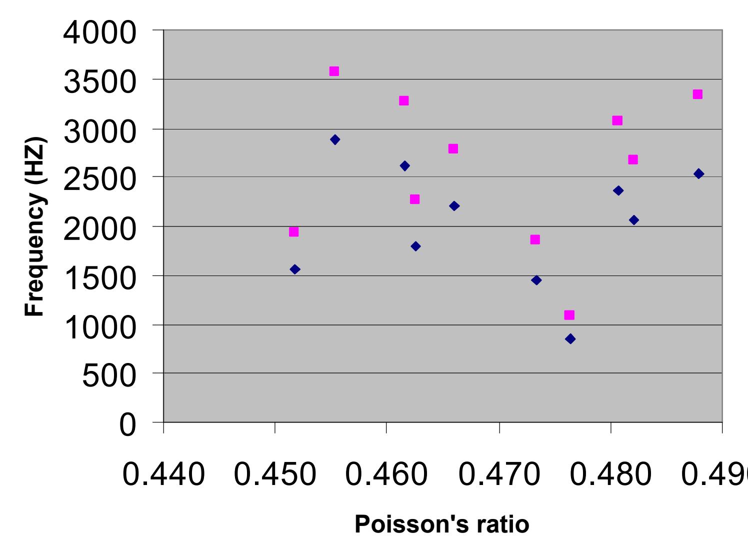
Axial mode frequency interval is [1088.1,3580.37] Hz.

Ten samples only used for initial study: need to use more

Strong linear correlation between E and shear/axial frequencies

Low correlation between ν and shear/axial frequencies





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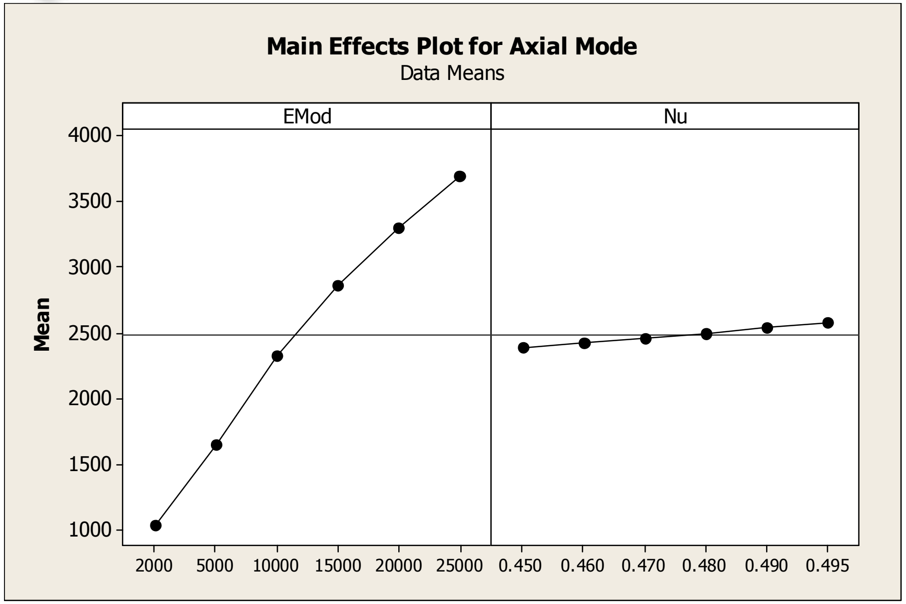
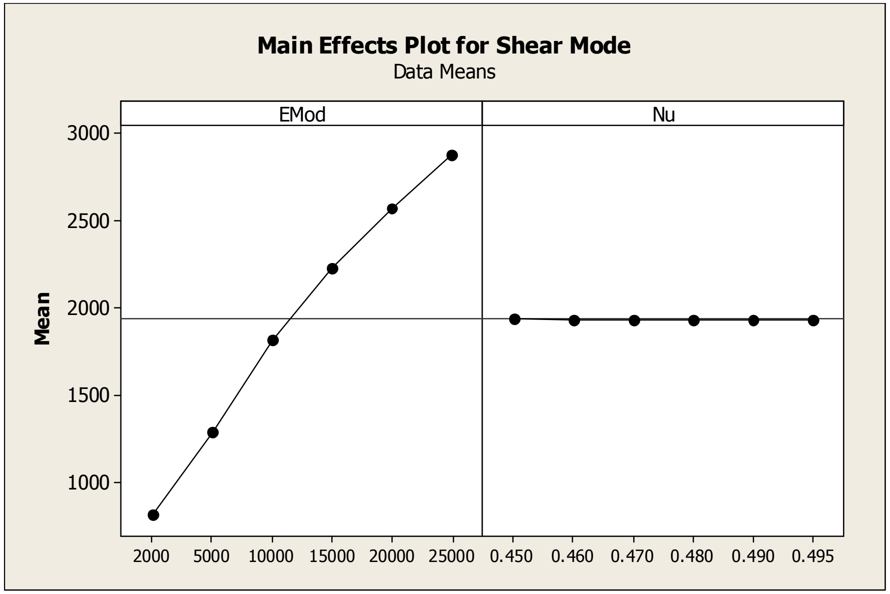
Further Analysis: Main Effects Analysis





- **Orthogonal array/main effects analysis verifies what we saw with sampling: output interval is dominated by E, not ν.**
- **Added 30 more samples, shear mode interval is [845.6, 2878.0] Hz and axial mode interval is [1088.1, 3696.0] Hz.**
- **In practice, want to use more samples (10*D, where D is number of uncertain variables) to determine output interval.**

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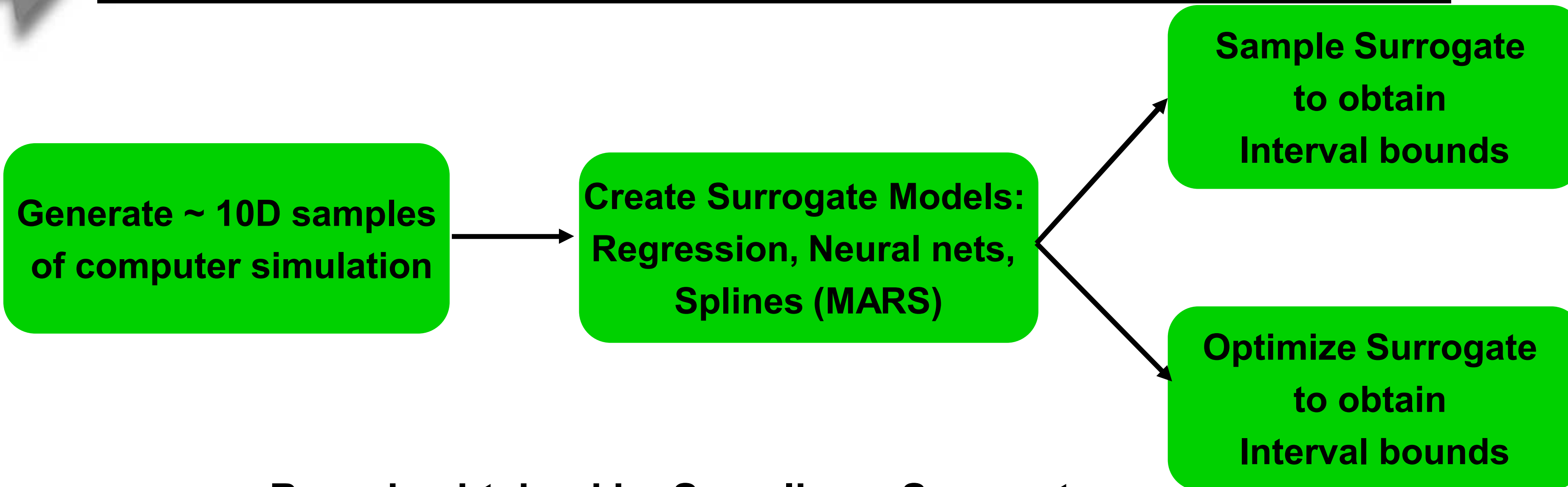
Interval Analysis: Surrogates



Bounds obtained by Sampling a Surrogate

	SHEAR MODE FREQUENCY		AXIAL MODE FREQUENCY	
Surrogate Type	Lower Bound	Upper Bound	Lower Bound	Upper Bound
Quadratic Regression	871.13	2849.90	1099.85	3775.50
Mars	816.03	2880.31	1028.04	3812.84
Neural Net	814.49	2893.26	1007.02	3807.57

Bounds obtained by Optimizing a Surrogate

	SHEAR MODE FREQUENCY		AXIAL MODE FREQUENCY	
Surrogate Type	Lower Bound	Upper Bound	Lower Bound	Upper Bound
Quadratic Regression	865.26	2852.54	1088.54	3791.74
Mars	816.03	2882.92	1011.43	3829.90
Neural Net	772.30	2906.90	993.58	3831.86

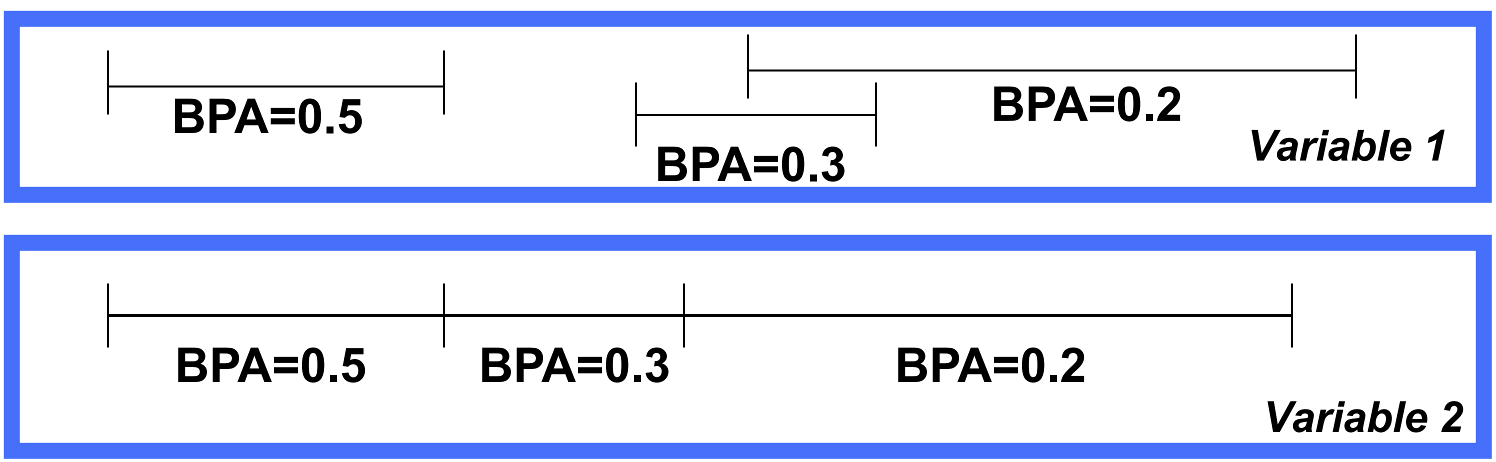
Surrogates in UQ

- **Very useful when you have an expensive computational simulation**
- **UQ analyses often require running thousands of simulations, so it is cheaper to do that on a surrogate**
- **You do need to understand something about the "goodness" of your surrogate. There are a variety of diagnostic metrics to help (R^2, mean absolute error, sum-squared error, cross-validation metrics or "leave one out", etc.)**
- **Although surrogates can be useful in interval analysis, often the surrogate is less accurate at bounds or endpoints: use caution**
- **Optimization can determine where minimum and maximum occur in input space:**

	Corresponding Bounding inputs [E,ν]	**Corresponding Bounding inputs [E,ν]**	**Corresponding Bounding inputs [E,ν]**	**Corresponding Bounding inputs [E,ν]**
Quadratic Regression	at 2000,0.494	at 25000,0.45	at 2000,0.45	at 25000,0.495
Mars	at 2000,0.468	at 25000,0.45	at 2000,0.45	at 25000,0.495
Neural Net	at 2000, 0.465	at 25000,0.465	at 2000,0.465	at 25000,0.495

Dempster-Shafer Theory

- Dempster-Shafer theory relaxes the assumptions of probability theory in situations where there is little information on which to evaluate a probability or when the information is nonspecific, ambiguous, or conflicting.
- Allows for conflicting expert opinions
- Allows the computational model to remain “black-box”
- Epistemic uncertain input variables are modeled as sets of intervals called 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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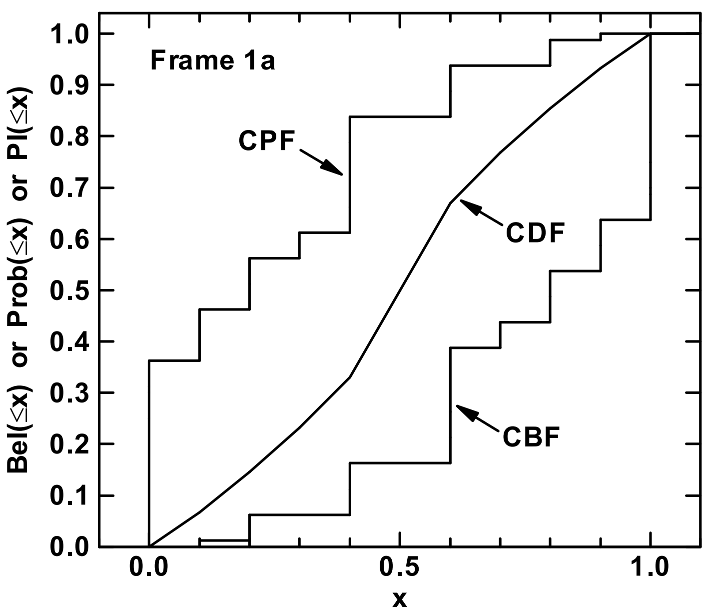
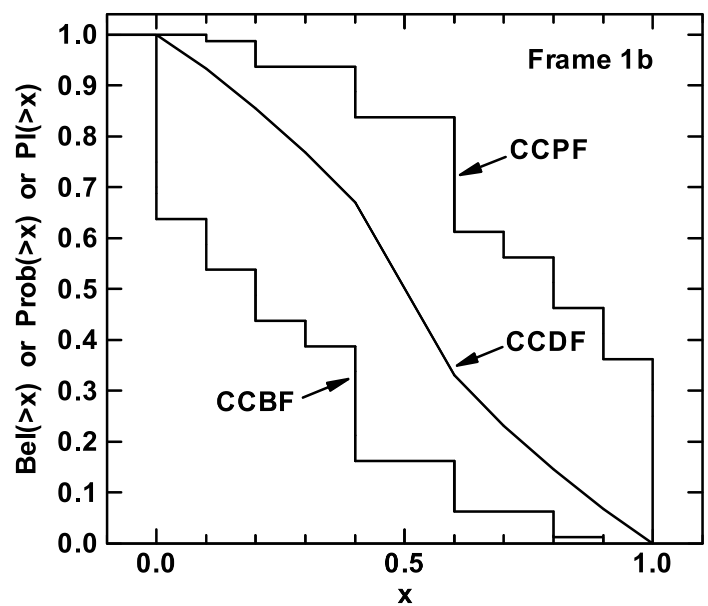
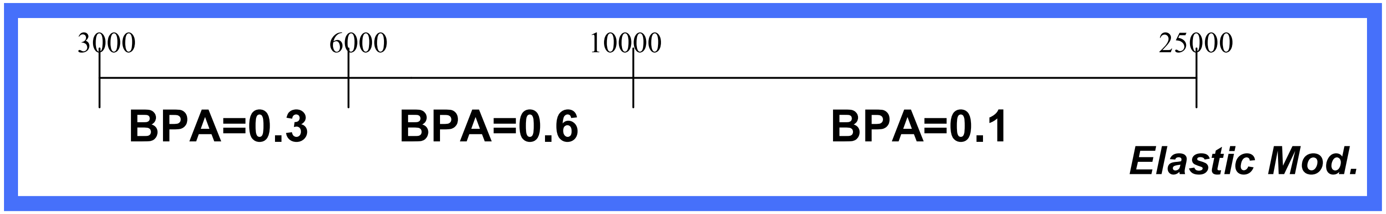
Dempster-Shafer Theory

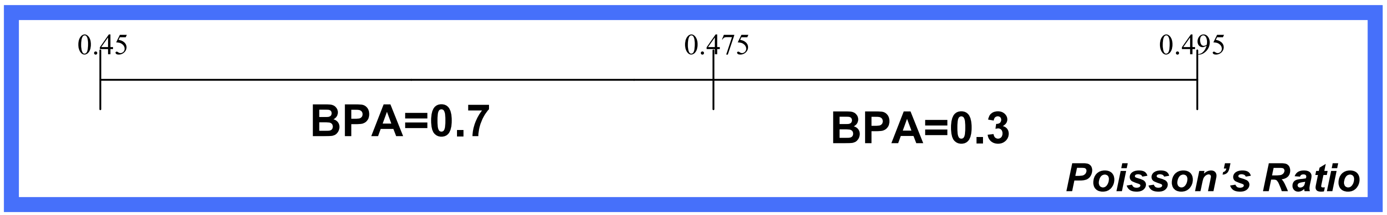
- Two output measures: belief and plausibility
- The intervals on the inputs are propagated to calculate belief (a lower bound on a probability value that is consistent with the evidence) and plausibility (an upper bound on a probability value that is consistent with the evidence).
- Together, belief and plausibility define an interval-valued probability distribution, not a single probability distribution.

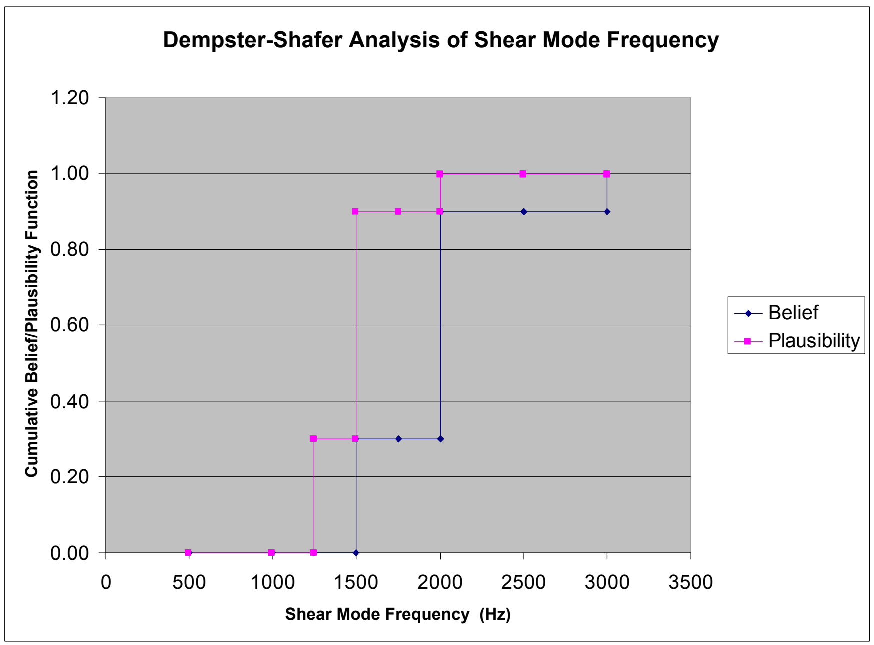


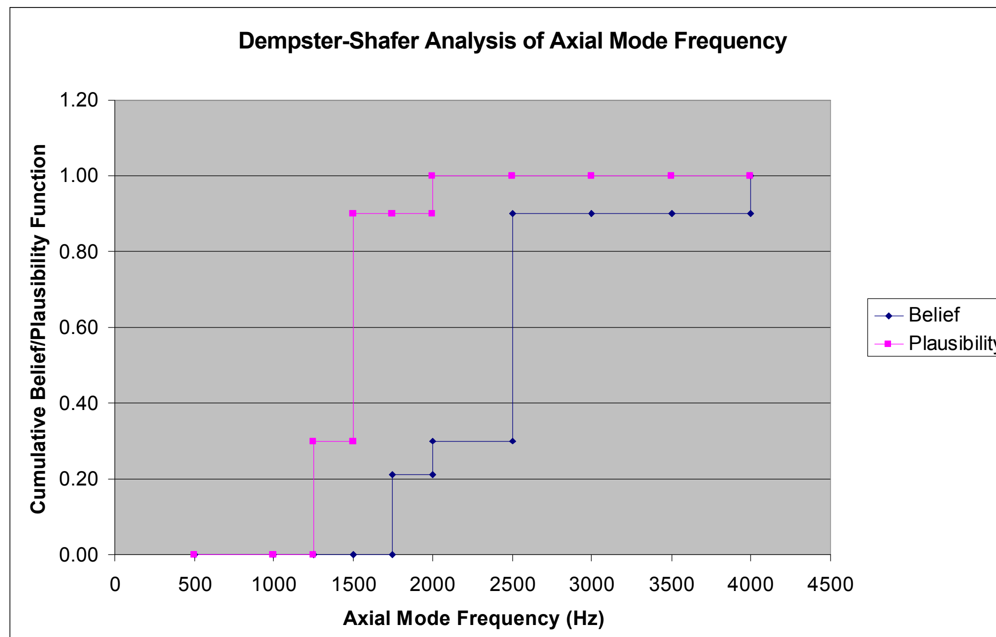


Dempster-Shafer Results





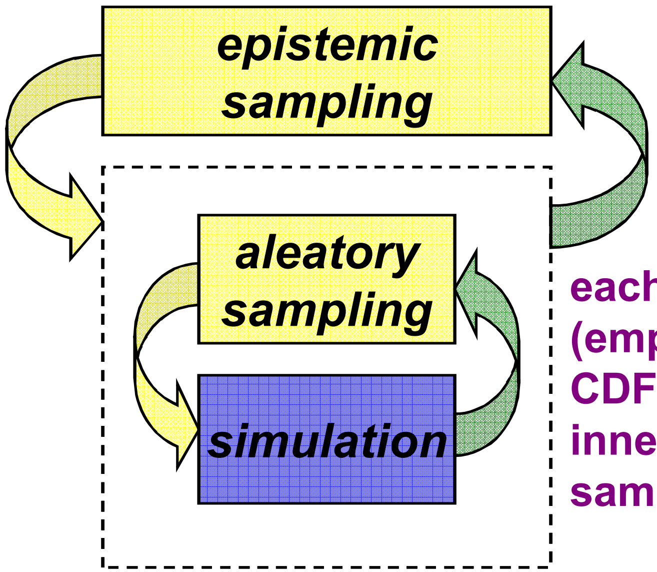




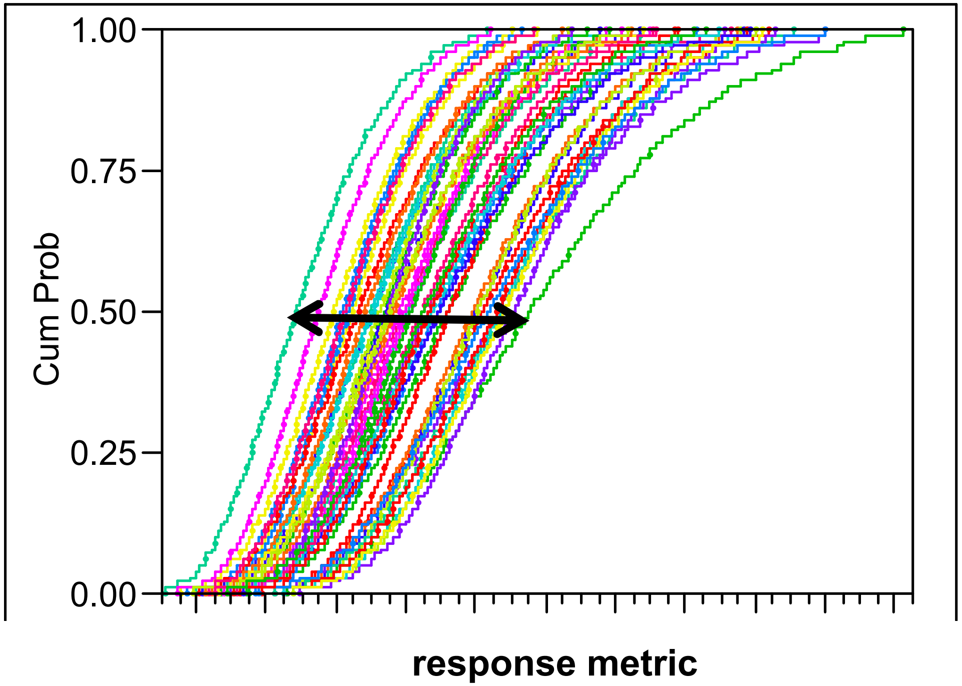
“Second-Order” Probability

- **Nested sampling technique which combines epistemic and aleatory uncertainty**
- **Frequently used in UQ studies and regulatory analyses (e.g. WIPP)**
- **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



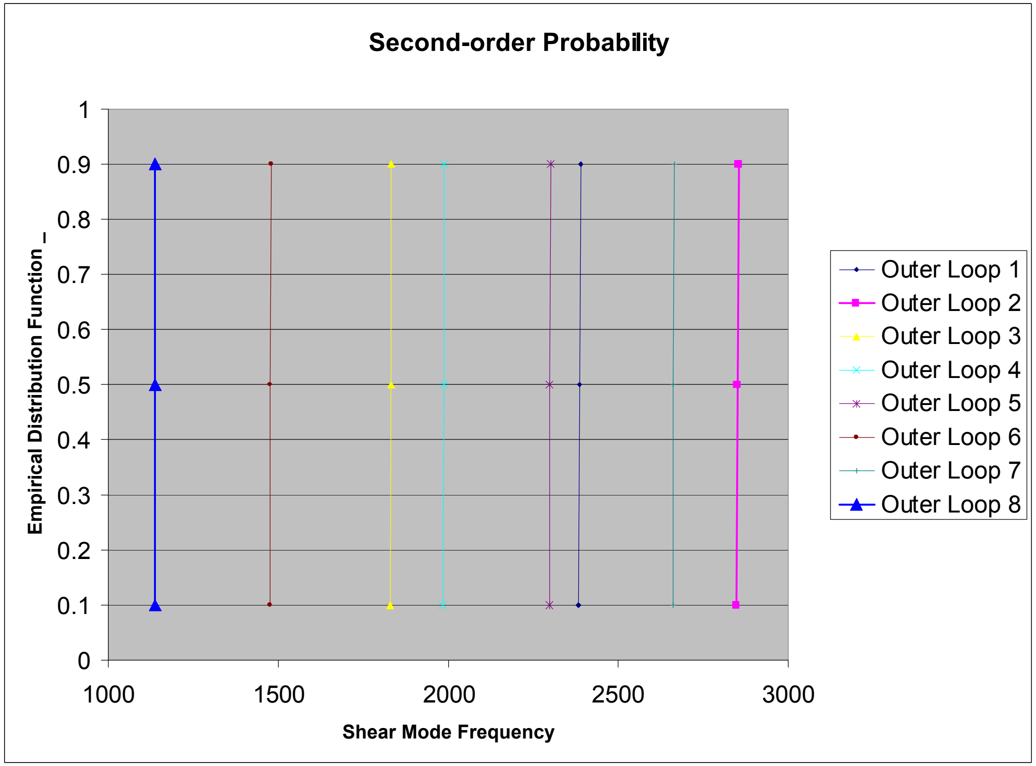
each discrete (empirical) CDF: 100 inner loop samples



“Envelope” of CDF traces represents response epistemic uncertainty

Second-Order Probability

- Treated E as the epistemic outer loop variable with bounds [2000,25000]
- Treated ν as the aleatory inner loop variable from a triangular distribution with mode 0.47, bounds [.45, .495]
- In practice, the epistemic variables often define parameters of aleatory distributions (e.g. aleatory variable is normal with an unknown mean, the unknown mean is defined by an epistemic interval). This is sometimes thought of as "distributions on distributions" similar to Bayesian analysis.



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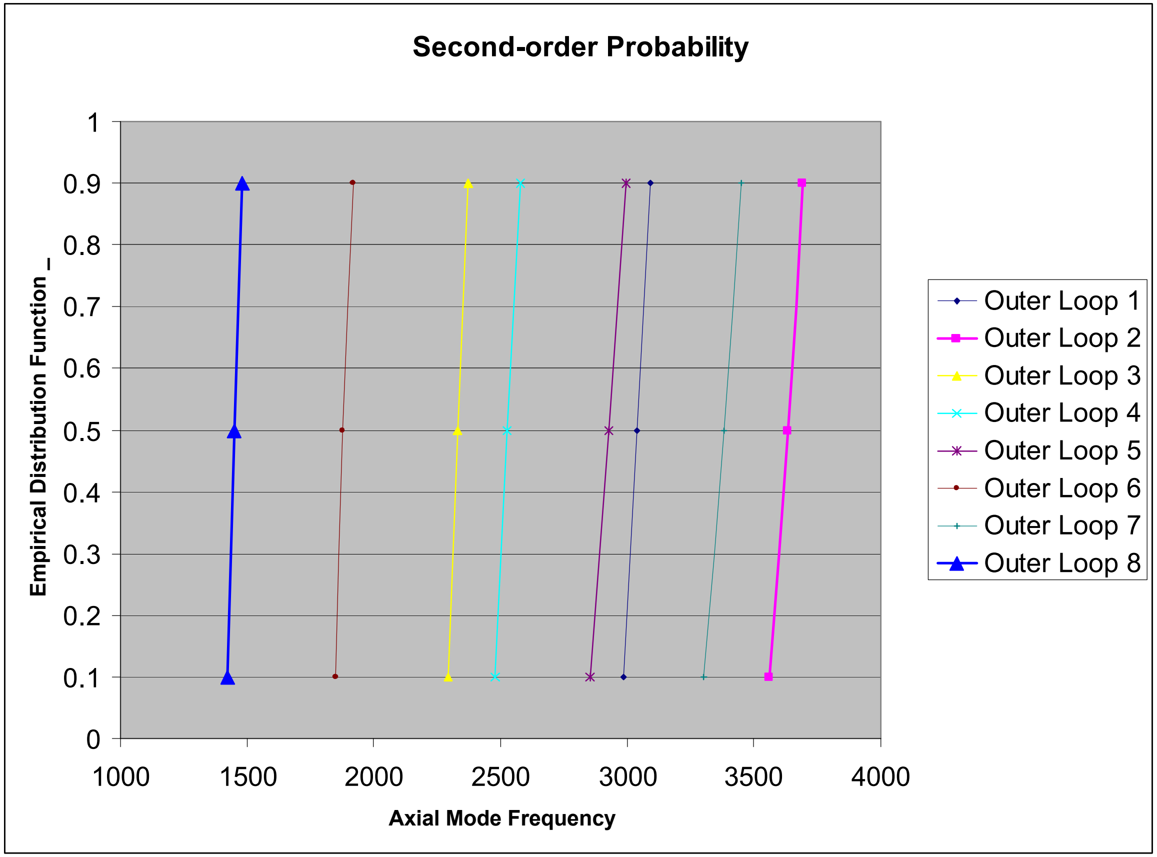
Second-Order Probability

- Generated 8 outer loop samples, 10 inner loop samples for a total of 80 samples
- In practice, you would need to run many more samples: this example is dominated by E and has a very linear response so the empirical distribution functions are nearly vertical



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Summary

- **When modeling uncertainty, if there are quantities about which you have very little information, or you have conflicting expert opinions, and/or you can improve your estimate with additional information, consider using an epistemic representation of uncertainty**
- **We have discussed 3 approaches for epistemic uncertainty: intervals, Dempster-Shafer theory, and second-order probability. There are many more (e.g. fuzzy set theory, imprecise probability, possibility theory, Bayesian methods).**

Summary

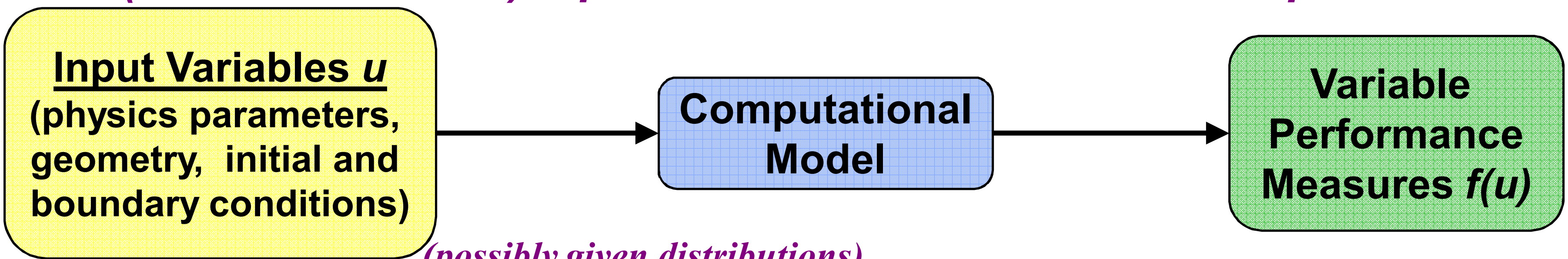
- **UQ methods (both aleatory and epistemic) are computationally expensive. Using surrogates can greatly help, but results obtained with surrogates need to be used with caution because the surrogate can be inaccurate**
- **The epistemic methods we discussed all place some type of bounds on the output:**
  - Interval analysis: Intervals in → Intervals out. Any value in the output interval is NOT equally likely (frequency interpretation), just possible.
  - Dempster-Shafer belief structure on the output. A particular percentile is bounded by a belief and plausibility
  - Second-order probability. Generate “families” or ensembles of CDFs which provide bounds on percentiles.
- **If output bounds are too large, perform sensitivity analysis to see where you can do additional testing/gather more information to reduce epistemic uncertainty.**

Questions?

Extra Slides

Uncertainty Quantification

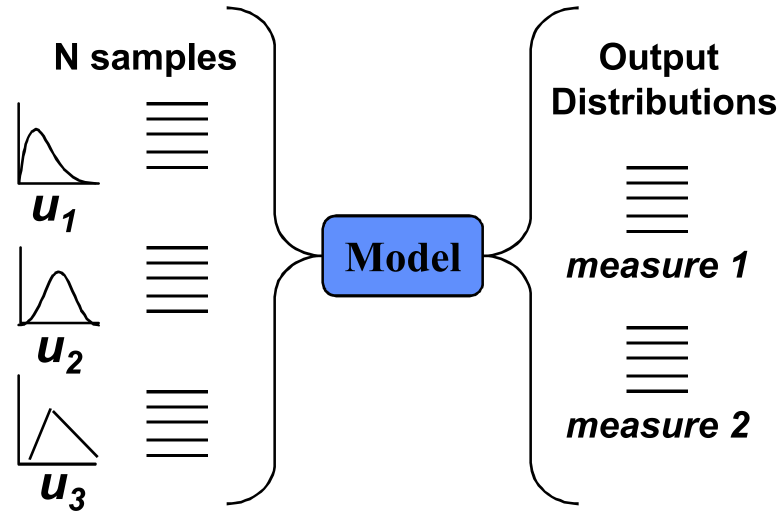
Forward propagation: quantify the effect that uncertain (nondeterministic) input variables have on model output



(possibly given distributions)

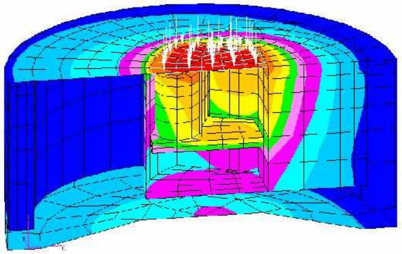
Potential Goals:

- **based on uncertain inputs, 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***



Typical method: Monte Carlo Sampling

DAKOTA Overview



iterative analysis…

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

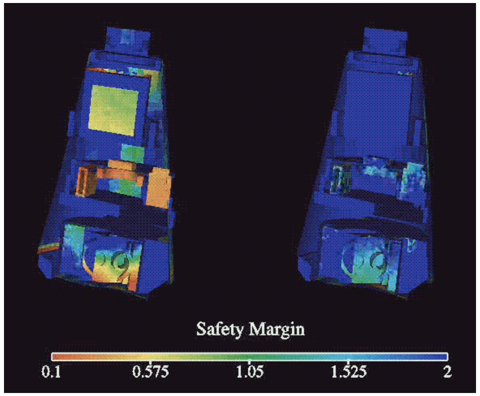
parameters
(design, UC, state)

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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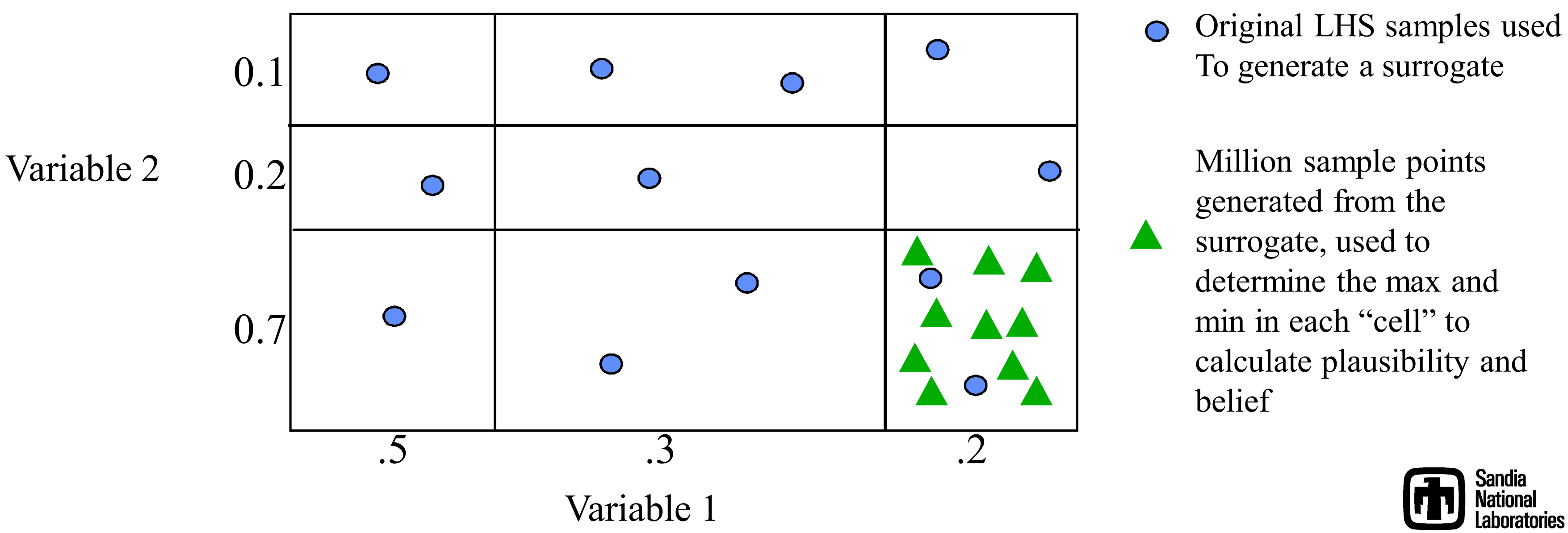
Epistemic Uncertainty Quantification

- 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



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

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