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From Uncertainty to Credibility: UQ Algorithms and Research Challenges

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Sandia National Laboratories
Optimization and Uncertainty Quantification

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2008 CSRI Summer Lecture Series
Sandia National Laboratories
Albuquerque, NM

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.

Route to Sandia

Ph.D., Computational and Applied Mathematics, NC State

- mathematics, statistics, computer science, immunology
- nondeterministic model calibration (HIV)
- internship at Fred Hutchinson Cancer Research Center

SNL since 2005 to fulfill goals:

- optimization focus (surprise: uncertainty quantification)
- develop algorithms; production software implementation in DAKOTA
- work with science/engineering application customers; *let their unmet needs drive research and software*

Outline

To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.

- **Ubiquitous computational simulation**
- **Why consider uncertainty quantification (UQ)**
- **Propagating uncertainty through models**
  - **Intro to UQ methods**
  - **Advanced UQ methods in DAKOTA**
- **Reliability-based MEMS design (OPT+UQ)**
- **Research challenges in electrical circuit UQ**

Slide credits: Mike Eldred, Laura Swiler, Barron Bichon, Genetha Gray, Bill Oberkampf, Matt Kerschen, others

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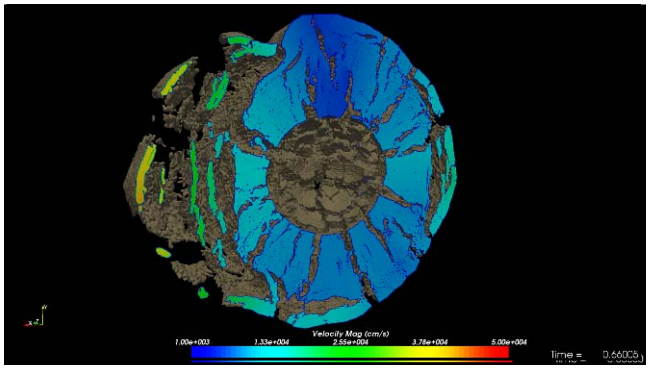
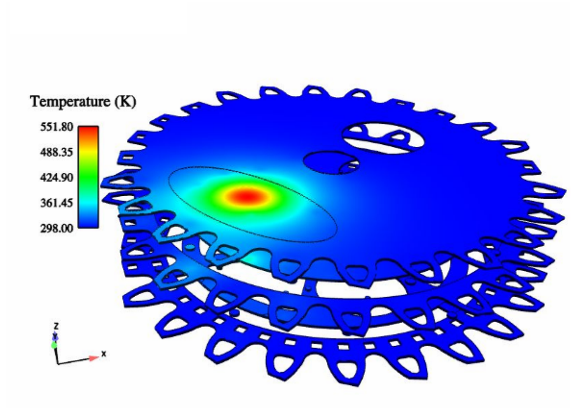
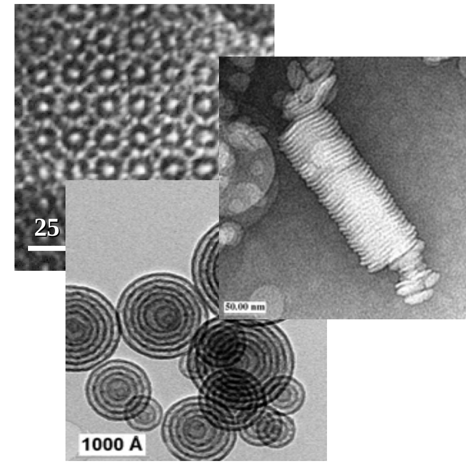
Sandia's Mission Focus Relies on Strong Science and Engineering



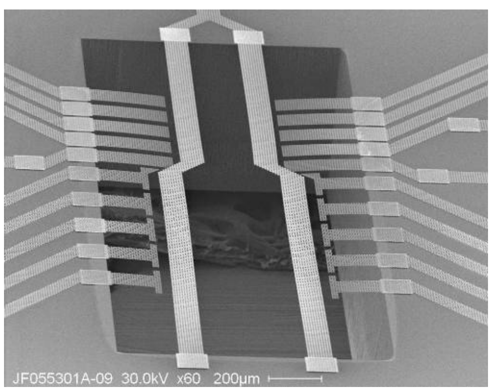
Computational and Information sciences



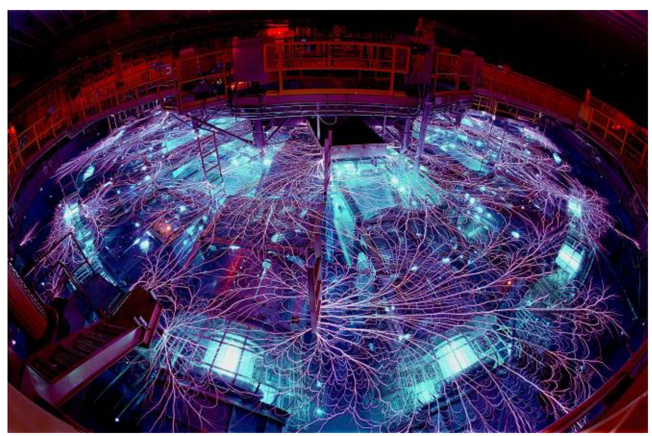
Engineering Sciences



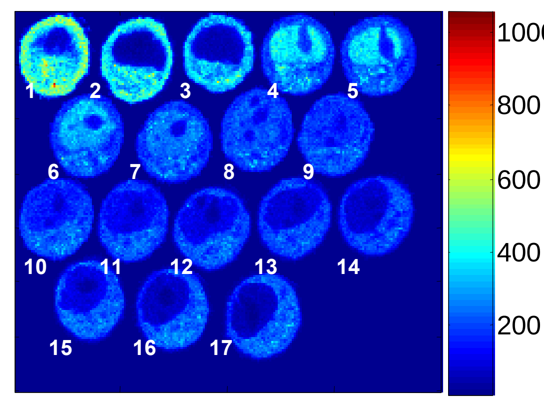
Materials Science and Technology



Microelectronics and Photonics

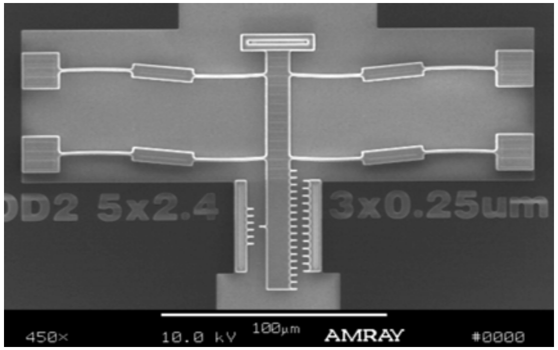


Pulsed Power

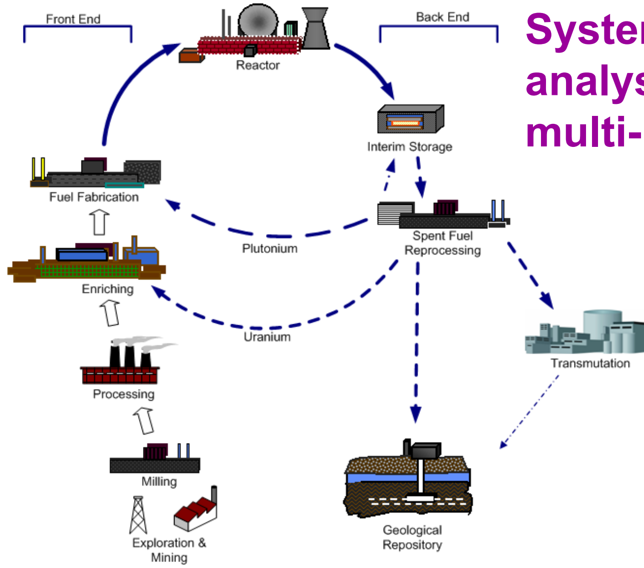


Bioscience

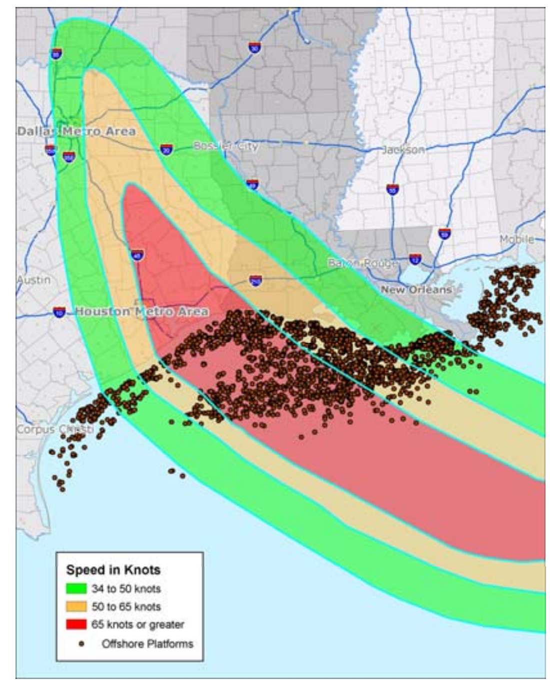
Computational Simulation



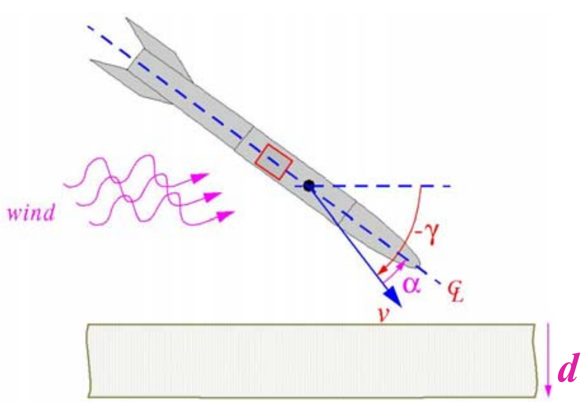
Micro-electro-mechanical systems (MEMS): quasi-static nonlinear elasticity, process modeling



Systems of systems analysis: multi-scale, multi-phenomenon

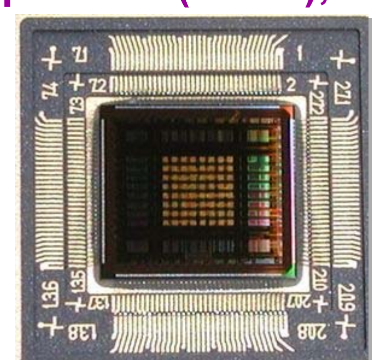


Hurricane Katrina: weather, logistics, economics, human behavior



Earth penetrator: nonlinear PDEs with contact, transient analysis, material modeling

Electrical circuits: networks, PDEs, differential algebraic equations (DAEs), E&M



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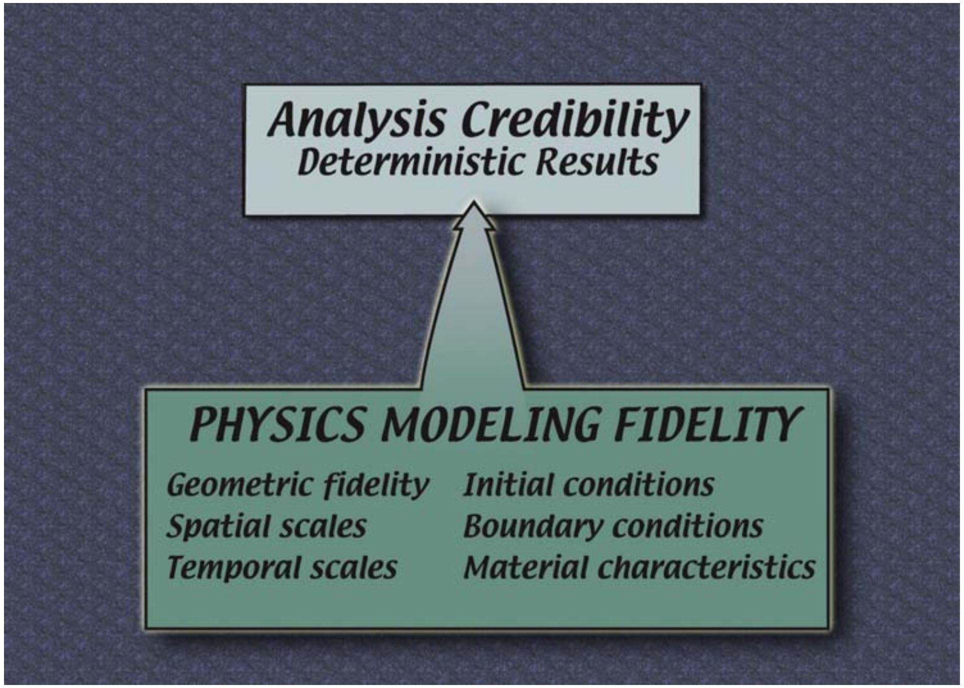
Credible Simulation

- **Ultimate purpose of modeling and simulation is (arguably) insight, prediction, and decision-making → *need credibility for intended application***



- **Historically: primary focus on *modeling fidelity***

Graphic credit: Bill Oberkampf

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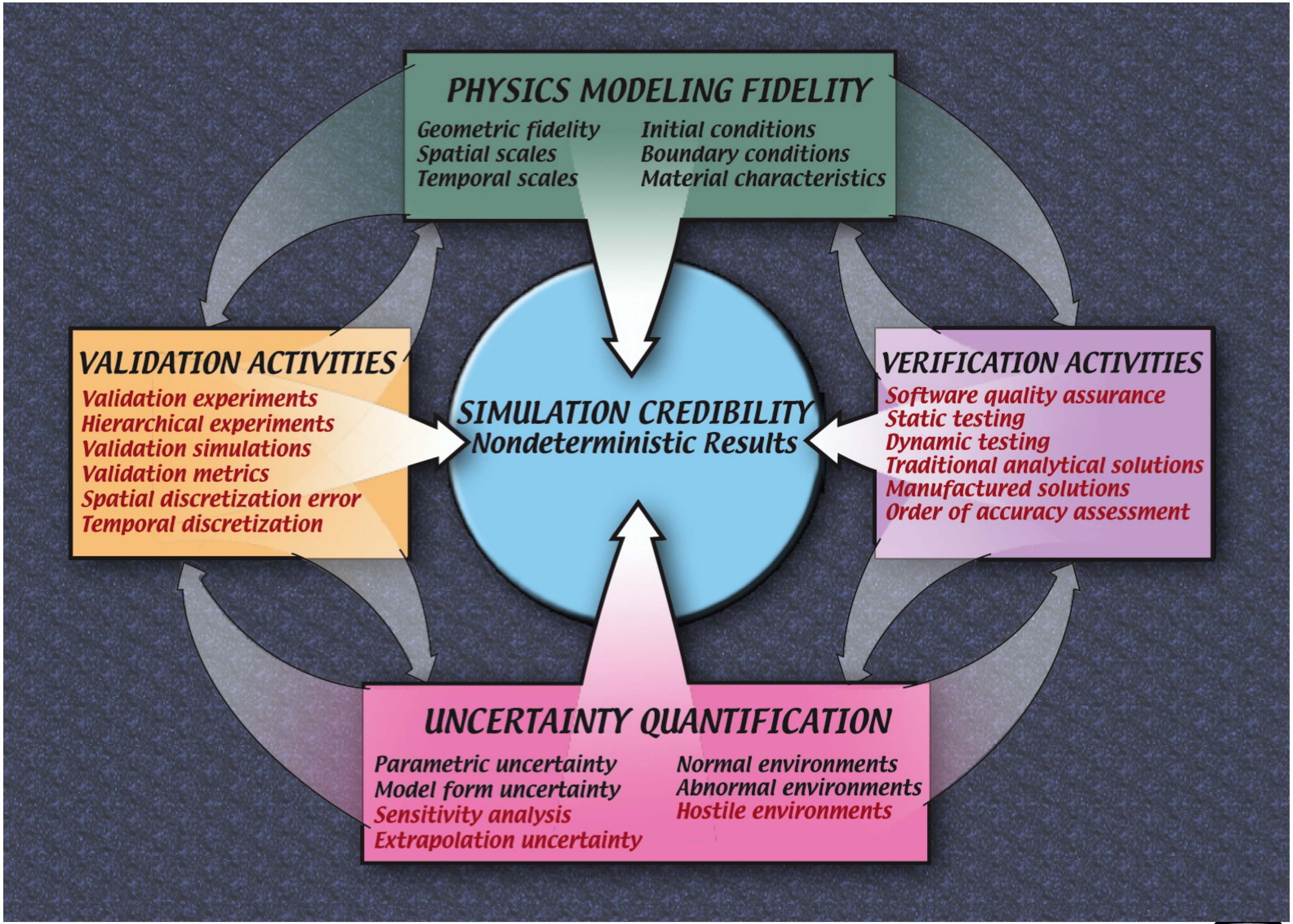
Credible Simulation: Beyond Nominal



Slide credit: Bill Oberkampf

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Verification & Validation

- **Verification: "Are we solving the equations correctly?"**
  - mathematics/computer science issue: Is our mathematical formulation and software implementation of the physics model correct?
  - *code verification* (software correctness);
    solution verification (e.g., exhibits proper order of convergence)

- **Validation – "Are we solving the right equations?"**
  - a disciplinary science issue: is the science (physics, biology, etc.) model sufficient *for the intended application?* Involves *data and metrics*.

Related concepts:

- **Sensitivity Analysis (SA): both local and global**
  - How do code outputs vary with respect to changes in code inputs?

- **Uncertainty Quantification (UQ):**
  - What are the probability distributions on code outputs, given the probability distributions on my code inputs? Unknown input distributions?

- **Quantification of margins and uncertainties (QMU):**
  - How "close" are my code output predictions (incl. UQ) to the system's required performance level?

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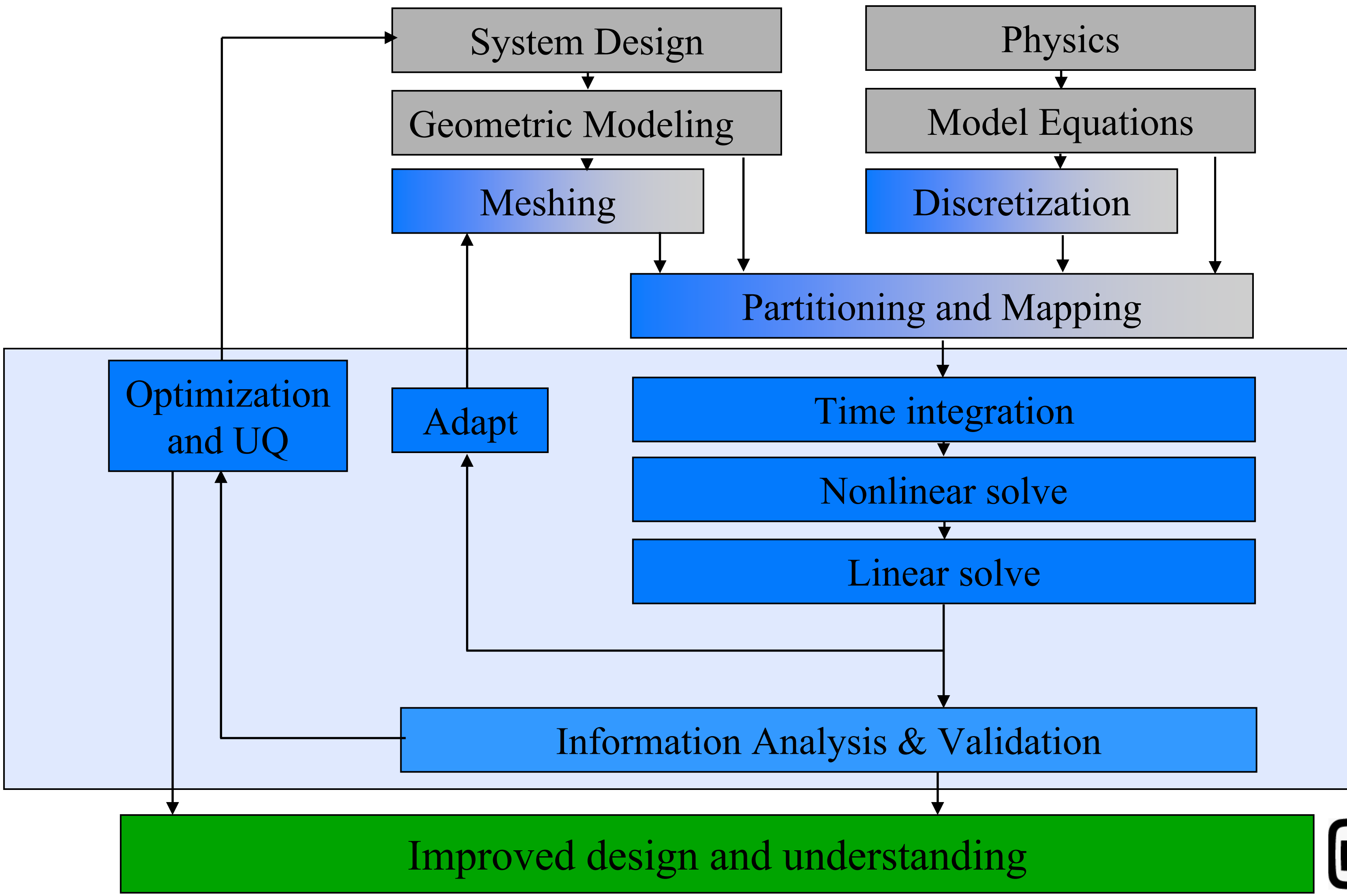
Algorithms for Computational Modeling & Simulation

Are you sure you don't need verification?!



Uncertainty Quantification

- **A single optimal design or nominal performance prediction is often insufficient for**
  - **decision making / trade-off assessment**
  - **validation with experimental data ensembles**
- ***Need to make risk-informed decisions, based on an assessment of uncertainty***

Uncertainties to Quantify

A partial list of uncertainties affecting computational model results

- physics/science parameters
- statistical variation, inherent randomness
- model form / accuracy
- operating environment, interference
- initial, boundary conditions; forcing
- geometry / structure / connectivity
- material properties
- manufacturing quality
- experimental error (measurement error, measurement bias)
- numerical accuracy (mesh, solvers); approximation error
- human reliability, subjective judgment, linguistic imprecision

Categories of Uncertainty

(Often useful distinctions, but not always a clear line between them)

- **Aleatory**
  - **Inherent variability (e.g., in a population)**
  - **Irreducible uncertainty – can't reduce it by further knowledge**

- **Epistemic** *(not in this talk, though a crucial research area)*
  - **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**

- **In practice, people try to transform or translate uncertainties to the aleatory type and perform sampling and/or parametric analysis**

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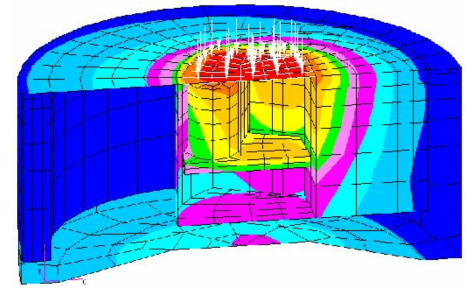
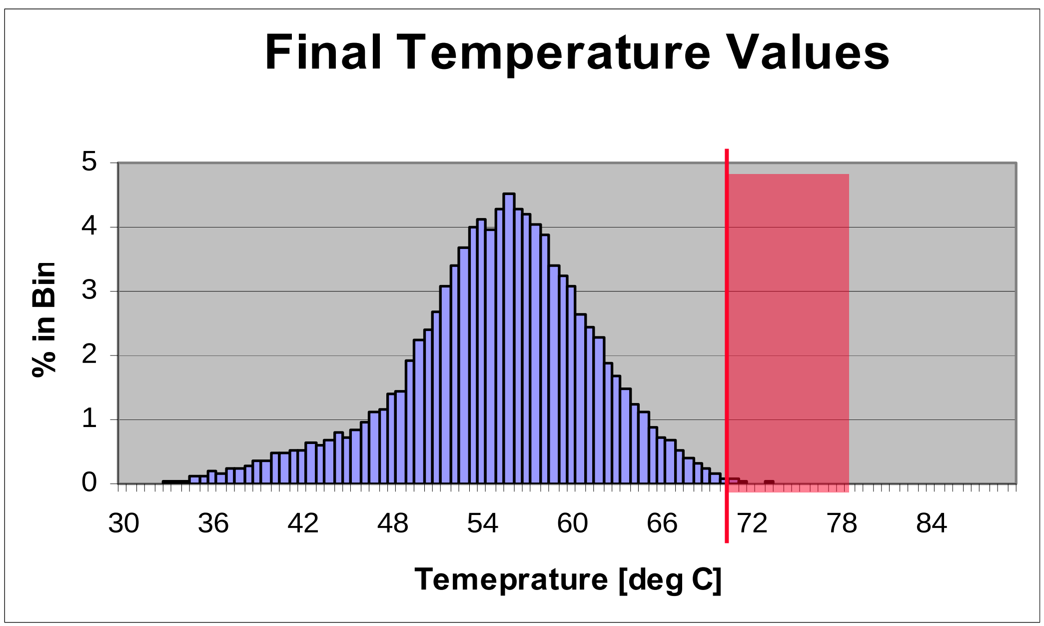
Uncertainty Quantification Example

- **Device subject to heating** (experiment or computational simulation)
- **Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by** $u_1, \ldots, u_N$
- **Response temperature** $f(u)=T(u_1, \ldots, u_N)$ **calculated by heat transfer code**





Given distributions of $u_1,\ldots,u_N$***, UQ methods calculate statistical info on outputs:***

- **Probability distribution of temperatures**
- **Correlations (trends) and sensitivity of temperature**
- **Mean(*T*), StdDev(*T*), Probability(**$T \geq T_{critical}$**)**

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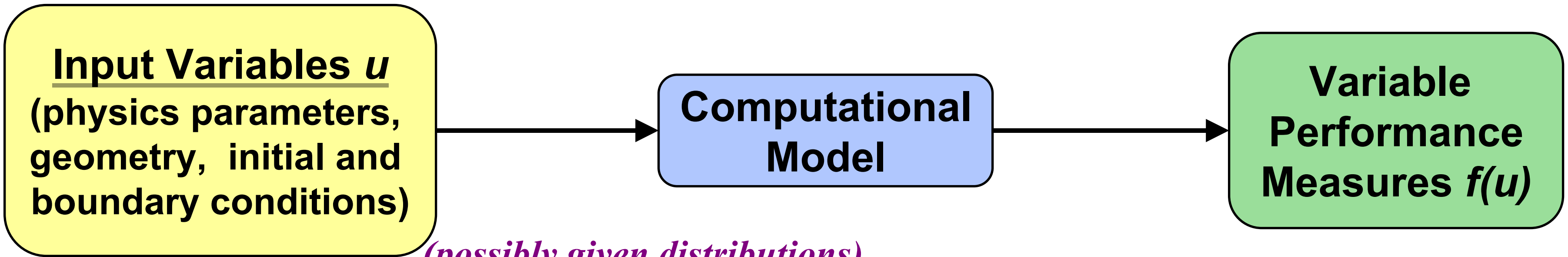
Uncertainty Quantification

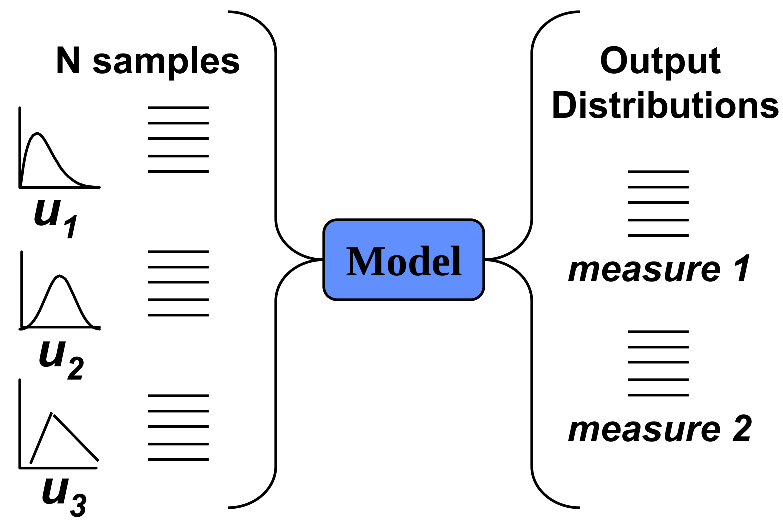
Forward propagation: quantify the effect that uncertain (nondeterministic) input variables have on model output



(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

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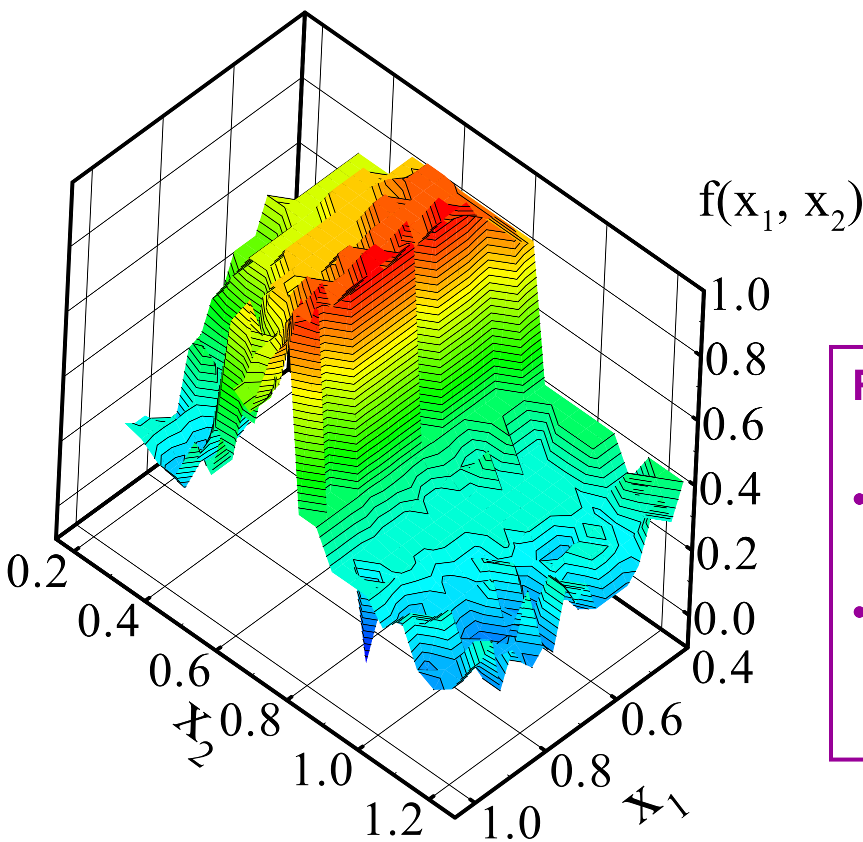
Challenges to This Process

- Engineering application: propagate variability through a computer model.
- Need statistics of response function "f", e.g., μ_f, σ_f, Prob[f > $f_{critical}$]
- Characteristics of response function:
  - input parameters specified by probability density functions
  - no explicit function for $f(x_1,x_2)$
  - expensive to evaluate $f(x_1,x_2)$ and may fail to calculate
  - limited number of samples
  - noisy / non-smooth



Research Question:
Which is more accurate?

- compute statistics from the $f(x_1,x_2)$ sample values, or
- construct an approximation model based on the $f(x_1,x_2)$ values and then compute statistics from the model?

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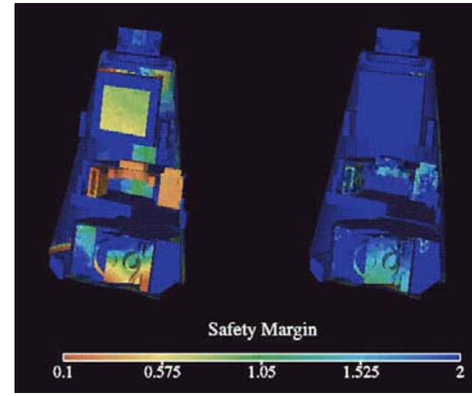
DAKOTA Motivation

Goal: perform iterative analysis on (potentially massively parallel) simulations to answer fundamental engineering questions:

- **What is the best performing design?**
- **How safe/reliable/robust is it?**
- **How much confidence do I have in my answer?**



Nominal **Optimized**

DAKOTA
optimization, sensitivity analysis, parameter estimation, uncertainty quantification

parameters (design, UC, state)

response metrics

Computational Model (simulation)

- **Black box:** any code: mechanics, circuits, high energy physics, biology, chemistry
- **Semi-intrusive:** Matlab, ModelCenter, Python SIERRA multi-physics, SALINAS, Xyce

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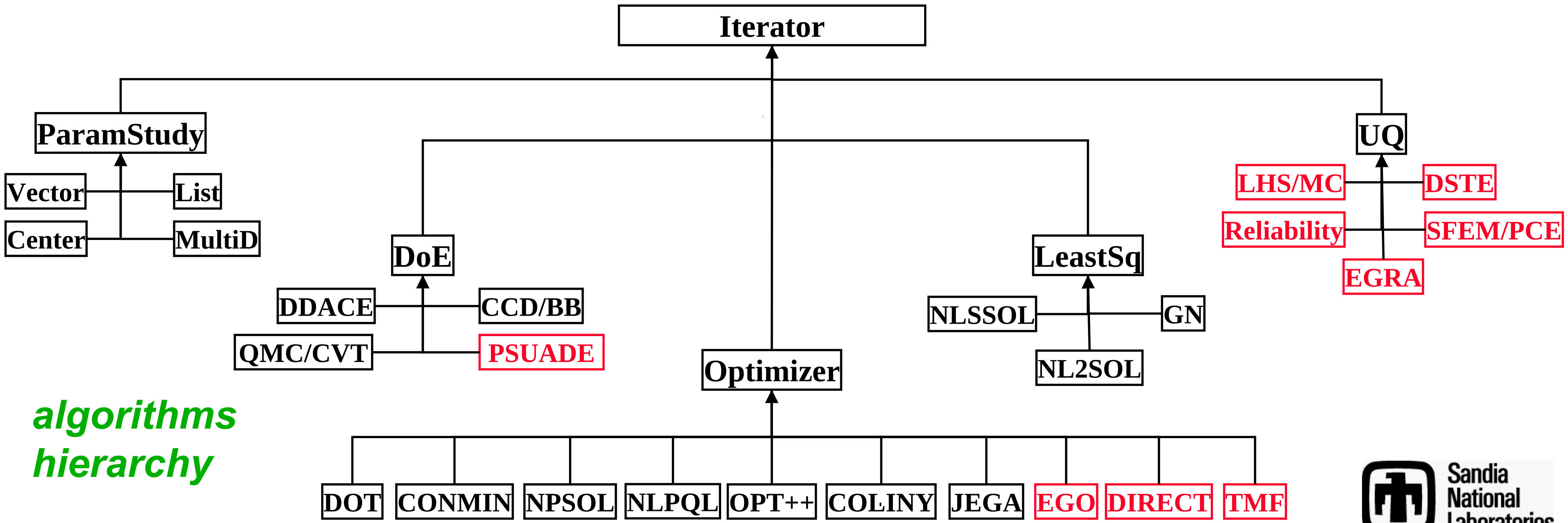
DAKOTA C++/OO Framework Goals

- **Unified software infrastructure:** reuse tools and common interfaces; *integrate commercial, open-source, and research algorithms*
- **Enable algorithm R&D**, e.g., for non-smooth/discontinuous/multimodal responses, probabilistic analysis and design, mixed variables, unreliable gradients, costly simulation failures
- **Facilitate scalable parallelism:** ASCI-scale applications and architectures; *4 nested levels of parallelism possible*
- **Impact:** tool for DOE labs and external partners; broad application deployment; *free via GNU GPL* (>3000 download registrations)



algorithms hierarchy

Flexibility with Models & Strategies

DAKOTA models map inputs to response metrics of interest:

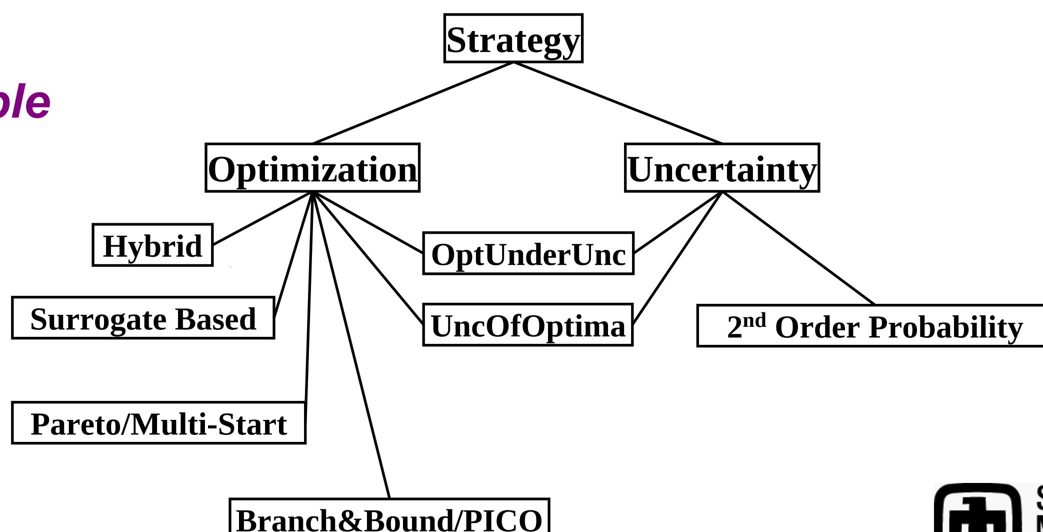
variables/parameters
- **design: continuous, discrete**
- **uncertain: (log)normal, (log)uniform, interval, triangular, histogram, beta/gamma, EV I, II, III**
- **state: continuous, discrete**

user application
(simulation)
system, fork, direct, grid

optional approximation (surrogate)
- **global (polynomial 1/2/3, neural net, kriging, MARS, RBF)**
- **local (Taylor); multipoint (TANA/3)**
- **hierarchical, multi-fidelity**

responses
- **functions: objectives, constraints, LSQ residuals, generic**
- **gradients: numerical, analytic**
- **Hessians: numerical, analytic, quasi**

DAKOTA strategies enable flexible combination of multiple models and algorithms.
- ***nested***
- ***layered***
- ***cascaded***
- ***concurrent***
- ***adaptive / interactive***



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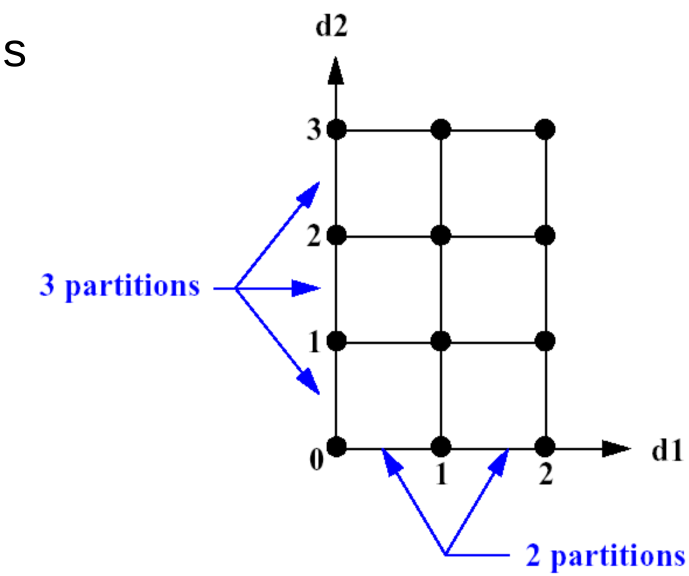
DAKOTA Sensitivity Analysis Methods

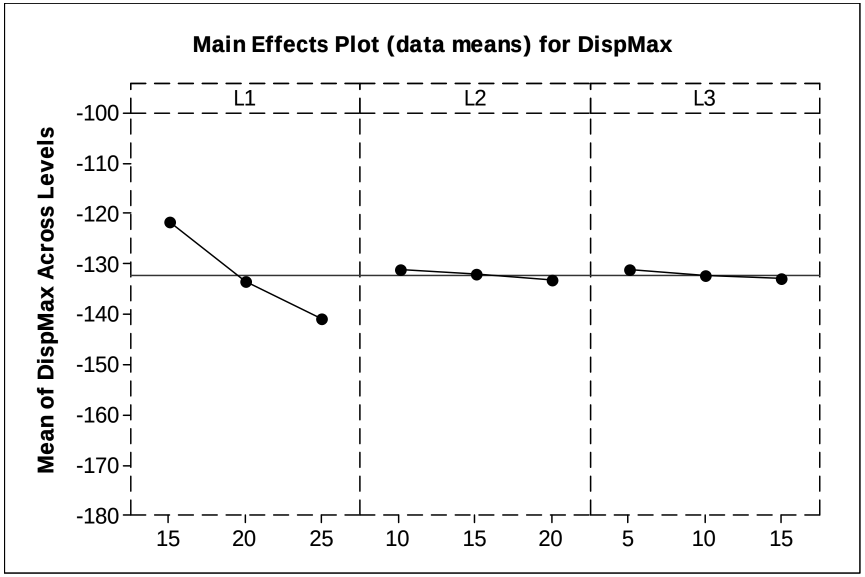
Sensitivity analysis techniques help determine which input variables are most important *(perhaps for which to refine uncertainty estimates)*

- **Parameter Studies**
  - Alter variables one at a time or on grid
  - Impractical in high dimension ***d*** ~ (partitions
- **Design of Computer Experiments (DACE) vs. Design of Experiments (DOE)**
  - Box-Behnken
  - Central Composite
  - Factorial and fractional designs
  - Orthogonal Arrays
- **Correlation Analysis**
  - Linear correlation
  - Variance-based decomposition
- **Morris One at a Time Sampling**



SA: Orthogonal Arrays

- **For each level of one factor, all levels of other factors occur equal number of times.**
- **Orthogonality: statistical independence between columns of the experimental design matrix (confounding factors cancel)**
- **Good for main effects,**
  terrible for variable interactions
- **Large OA databases available**



Exp. No	Var. 1	Var. 2	Var. 3	Var. 4	Var. 5	Var. 6	Var. 7
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	2	2
4	1	2	2	2	2	1	1
5	2	1	2	1	2	1	2
6	2	1	2	2	1	2	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

Main effects of 7 variables, each with 2 levels, in 8 samples!

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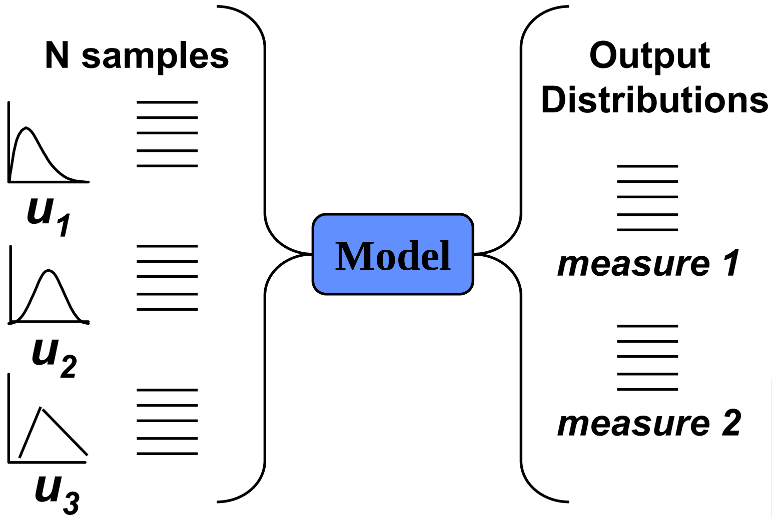
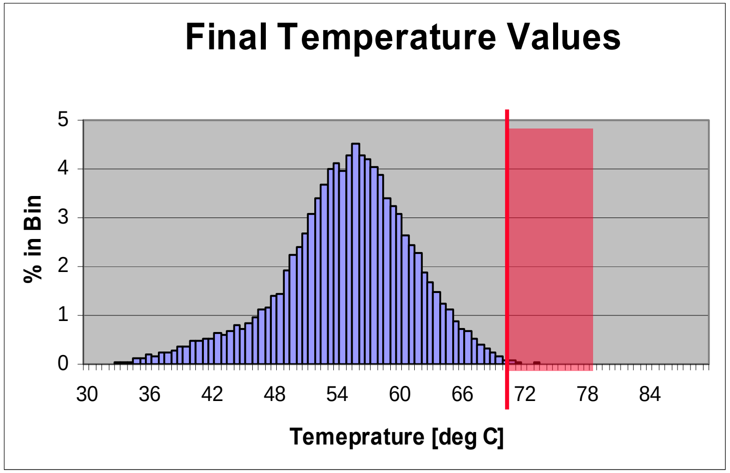
UQ: Sampling Methods

Given <u>distributions</u> of $u_1,\ldots,u_N$, UQ methods…



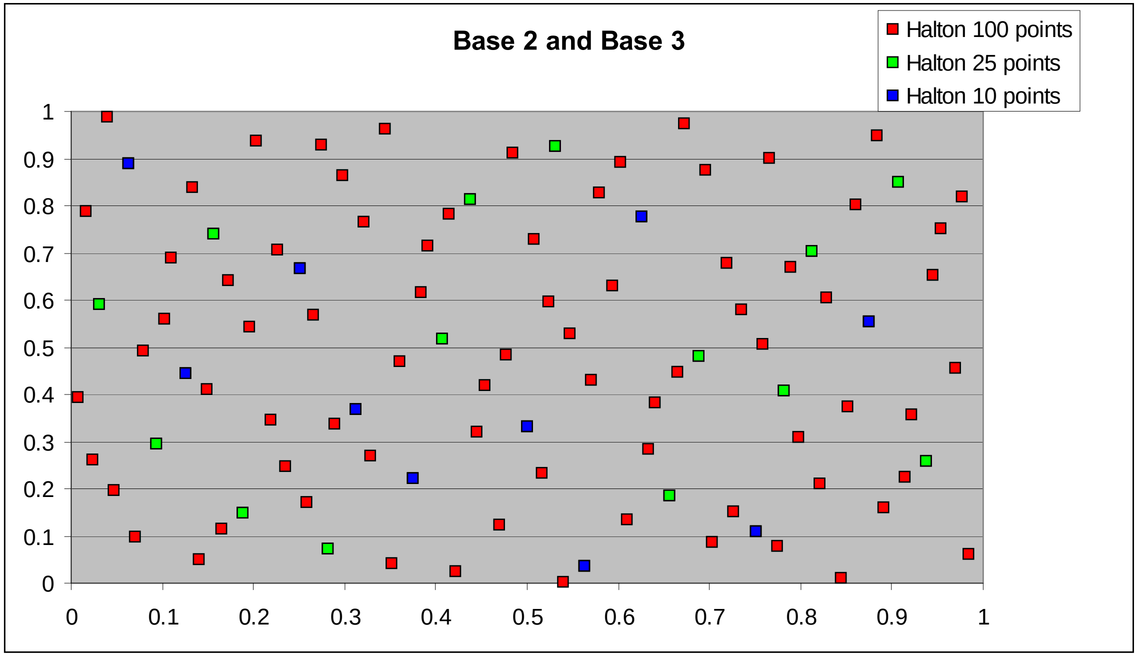
…calculate statistical info on outputs $T(u_1,\ldots,u_N)$



Quasi-Monte Carlo Sequences

- **Deterministic sequences from a series of prime bases**
- **Designed to produce uniform random numbers on the interval [0,1]**
- **Low discrepancy**
- **Example: Halton sequences**

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



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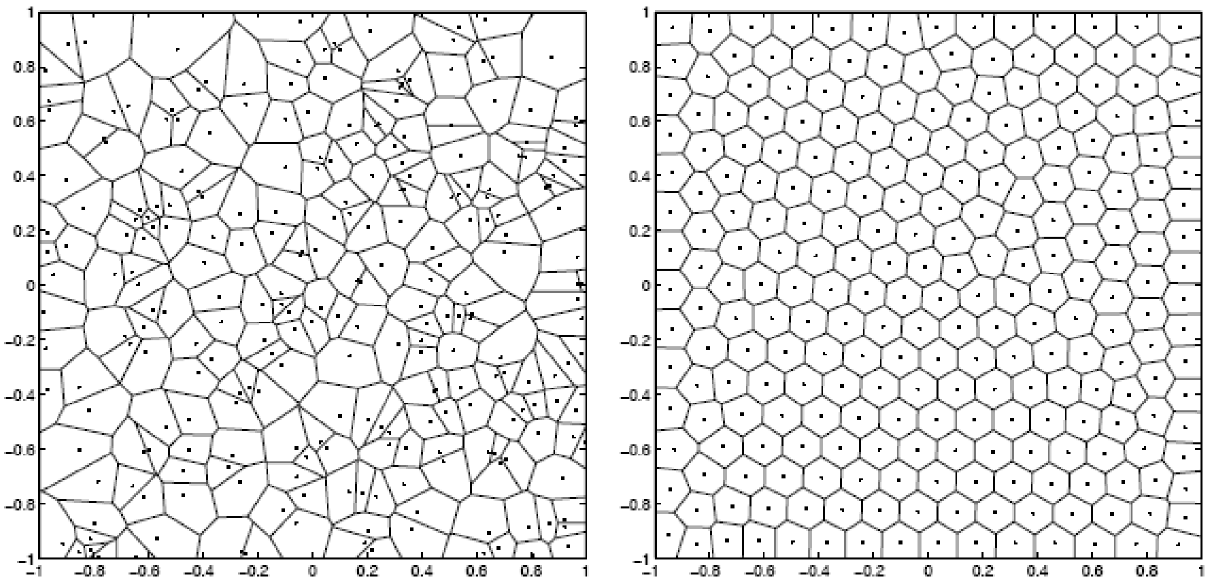
Centroidal Voroni Tessalation (CVT)

- Generates nearly uniform spacing over arbitrarily shaped parameter spaces (can also be used for non-uniform distributions)
- Origin: unstructured meshing for irregular domains
- Ideal for high dimensional volumetric sampling



Gunzburger, et al.: comparison of random sampling and CVT

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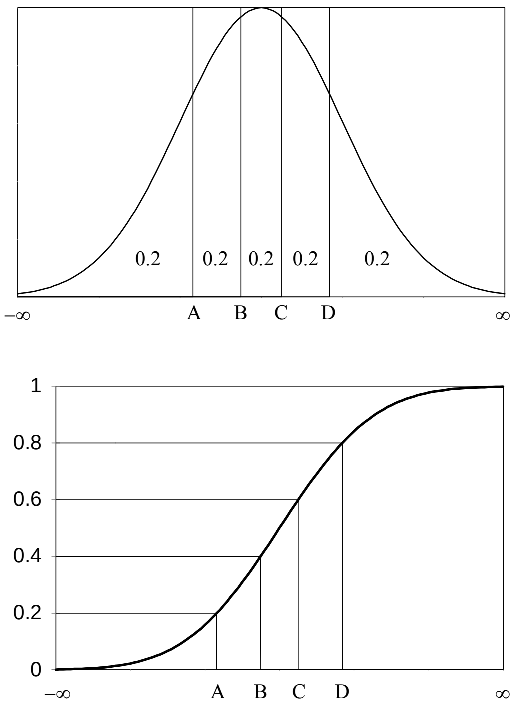
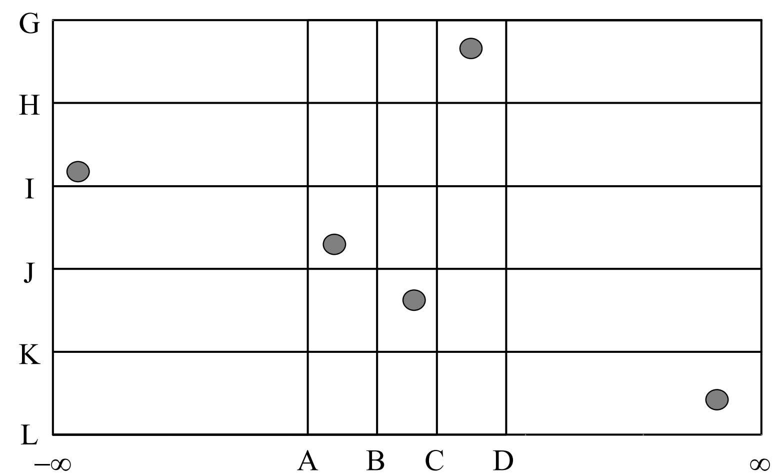
Latin Hypercube Sampling (LHS)

- **Specialized Monte Carlo (MC) sampling technique: workhorse method in DAKOTA / at Sandia**
- ***Stratified random sampling among equal probability bins*** **for all 1-D projections of an n-dimensional set of samples.**
- **McKay and Conover (early), restricted pairing by Iman**



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)

Generalized Polynomial Chaos Expansions

Approximate response stochasticity with Galerkin projection using multivariate orthogonal polynomial basis functions defined over standard random variables

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

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

$R(\xi) \approx f(u)$

- **Intrusive**
- **Nonintrusive: estimate response coefficients using sampling (expectation), quadrature/cubature (num integration), point collocation (regression)**

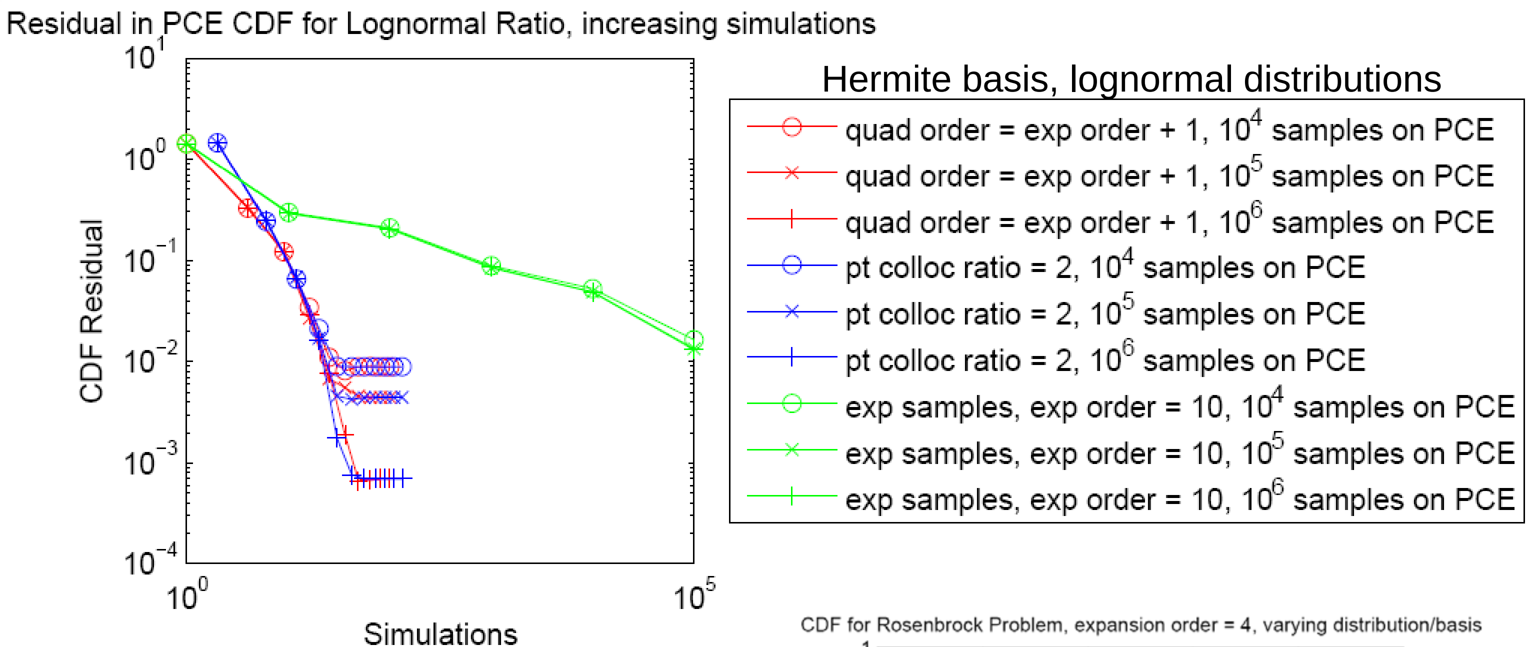
Wiener-Askey Generalized PCE with adaptivity

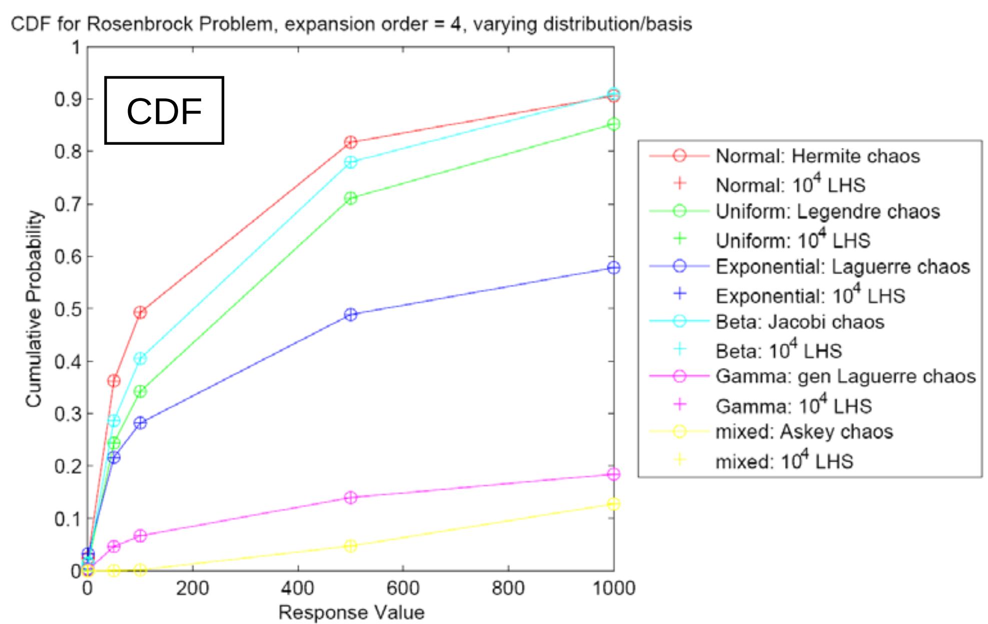
- Tailor basis: optimal basis selection leads to exponential convergence rates

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/integration order: adaptivity based on PC error estimates
  - Isotropic/anisotropic tensor-product quadrature & sparse grid Smolyak cubature

PCE: Fast Convergence





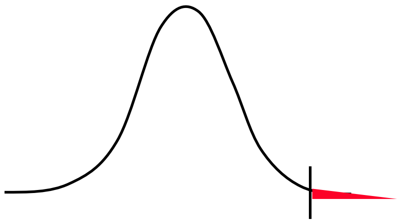
UQ Not Addressed Here

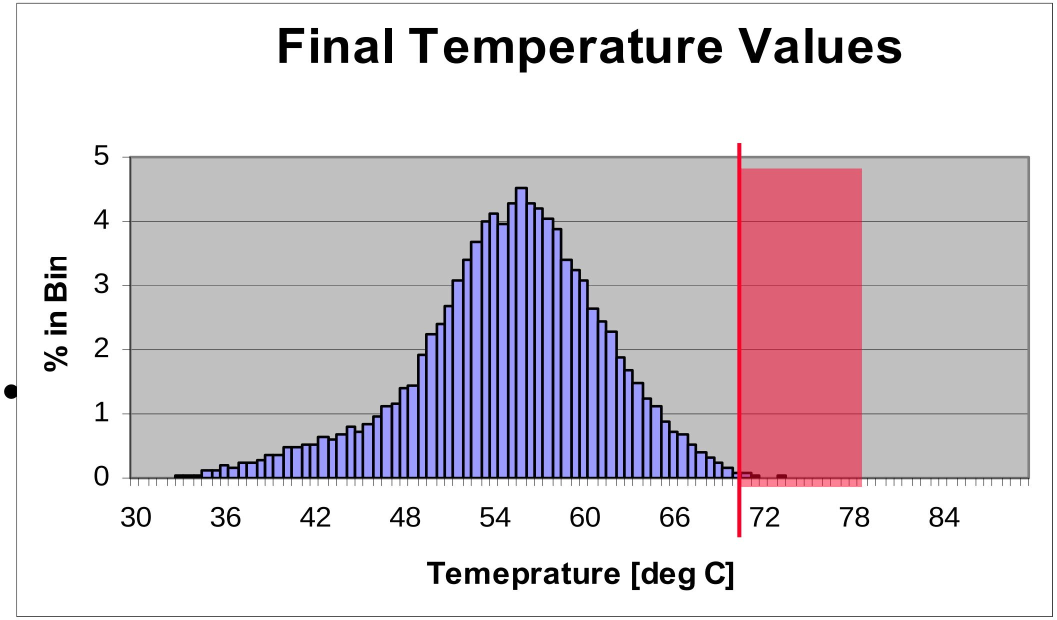
- *Efficient epistemic UQ (big research area)*
- Fuzzy sets (Zadeh)
- Imprecise Probability (Walley)
- Dempster-Shafer Theory of Evidence (Klir, Oberkampf, Ferson)
- Possibility theory (Joslyn)
- Probability bounds analysis (p-boxes)
- Info-gap analysis (Ben-Haim)

- *Production Bayesian analysis capability*
- Bayesian approaches: Bayesian belief networks, Bayesian updating, Robust Bayes, etc.
- Scenario evaluation

Calculating Probability of Failure

- ***Given uncertainty in materials, geometry, and environment, determine likelihood of failure Probability($T \geq T_{critical}$)***





- **Could perform 10,000 Monte Carlo samples and count how many exceed the threshold…**
- **Or directly determine input variables which give rise to failure behaviors by solving an optimization problem.**

By combining optimization, uncertainty analysis methods, and surrogate (meta-) modeling in a single framework, DAKOTA enables more efficient UQ.

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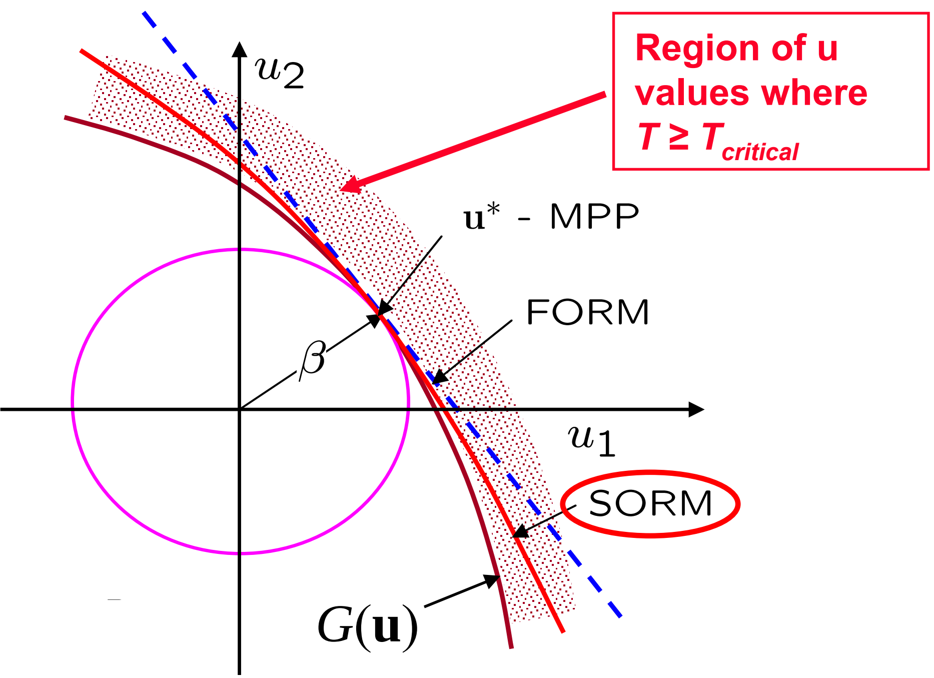
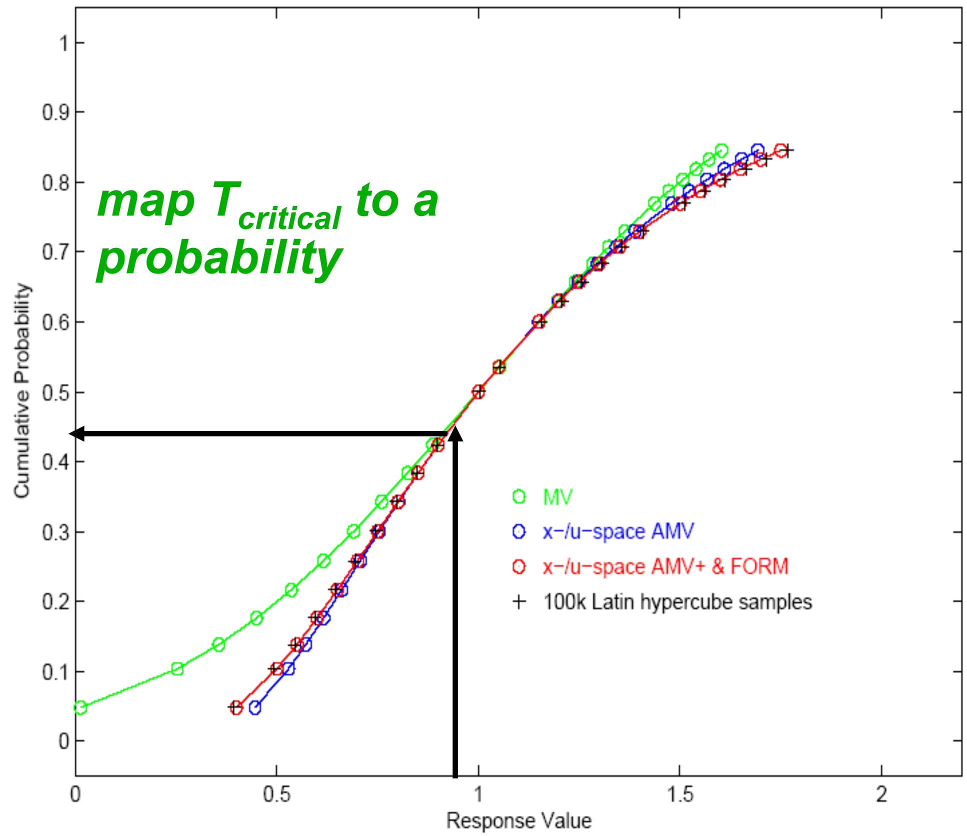
Analytic Reliability: MPP Search

Perform optimization **in uncertain variable space to determine Most Probable Point (of response or failure occurring) for** ***G(u) = T(u)*****.**

Reliability Index Approach (RIA)

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





Reliability: Algorithmic Variations

Many variations possible to improve efficiency, including in DAKOTA…

- **Limit state linearizations: use a local surrogate for the limit state *G(u)* during optimization in u-space (or x-space):**

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

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

u-space AMV^2+: $G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T (\mathbf{u} - \mathbf{u}^*) + \frac{1}{2}(\mathbf{u} - \mathbf{u}^*)^T \nabla_u^2 G(\mathbf{u}^*)(\mathbf{u} - \mathbf{u}^*)$

(could use analytic, finite difference, or quasi-Newton (BFGS, SR1) Hessians in approximation/optimization – results here mostly use SR1 quasi-Hessians.)

- **Integrations (in u-space to determine probabilities): may need higher order for nonlinear limit states**

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

2nd-order: $\left\{ p = \Phi(-\beta) \prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta \kappa_i}} \right.$

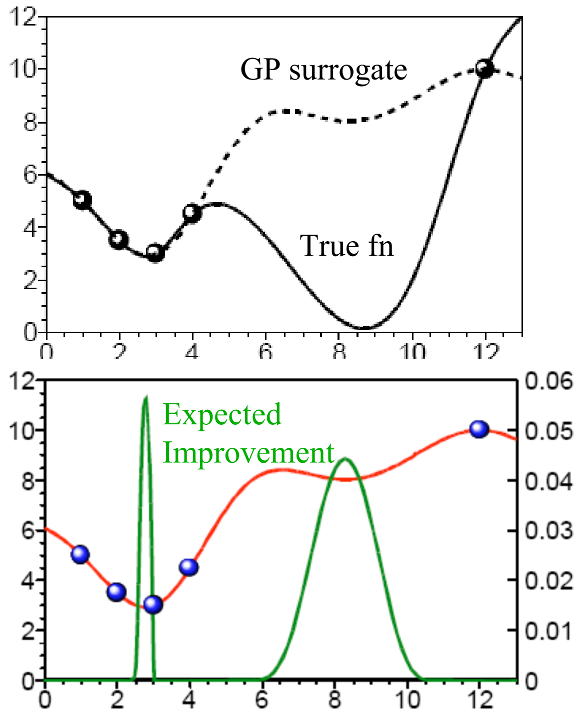
curvature correction

- **MPP search algorithm:** Sequential Quadratic Prog. (SQP) vs. Nonlinear Interior Point (NIP)
- **Warm starting (for linearizations, initial iterate for MPP searches):** speeds convergence when increments made in: approximation, statistics requested, design variables

Efficient Global Reliability Analysis

- **EGRA (B.J. Bichon) performs reliability analysis with EGO (Gaussian Process surrogate and NCSU DIRECT optimizer) coupled with Multimodal adaptive importance sampling for probability calculation.**

- **Created to address nonlinear and/or multi-modal limit states in MPP searches.**



From Jones, Schonlau, Welch, 1998

Efficient Global Reliability Analysis

- **EGRA** (B.J. Bichon) performs reliability analysis with EGO (Gaussian Process surrogate and NCSU DIRECT optimizer) coupled with Multimodal adaptive importance sampling for probability calculation.

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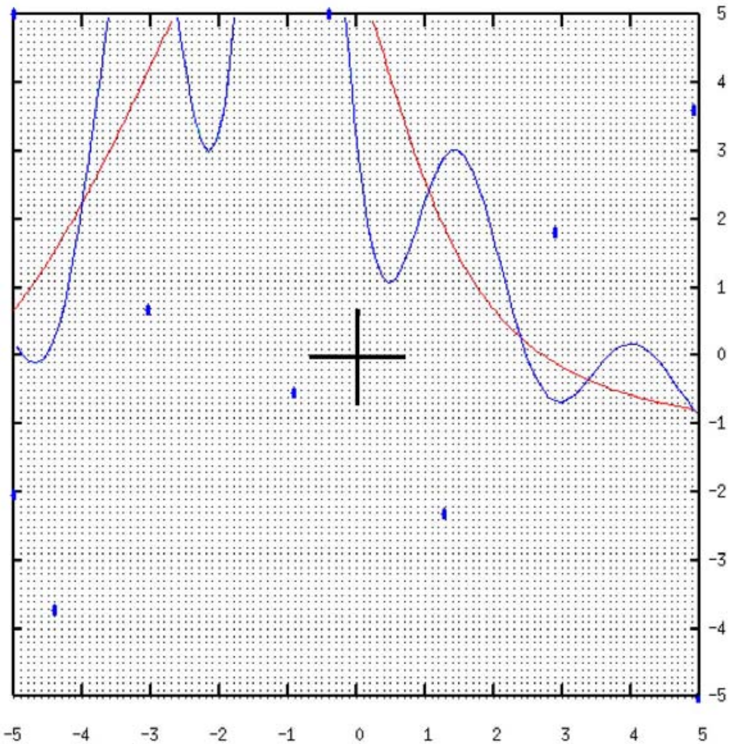
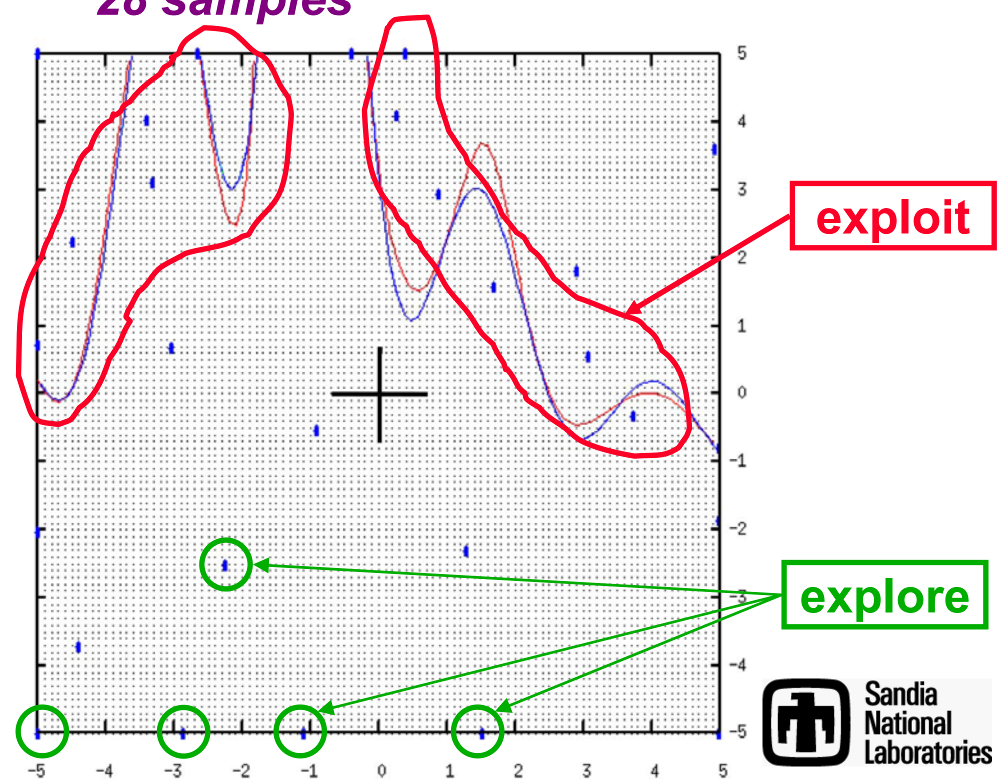
Gaussian process model of reliability limit state with

10 samples



28 samples



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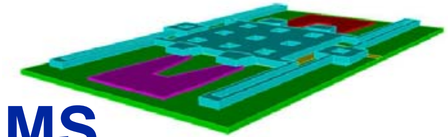
Outline

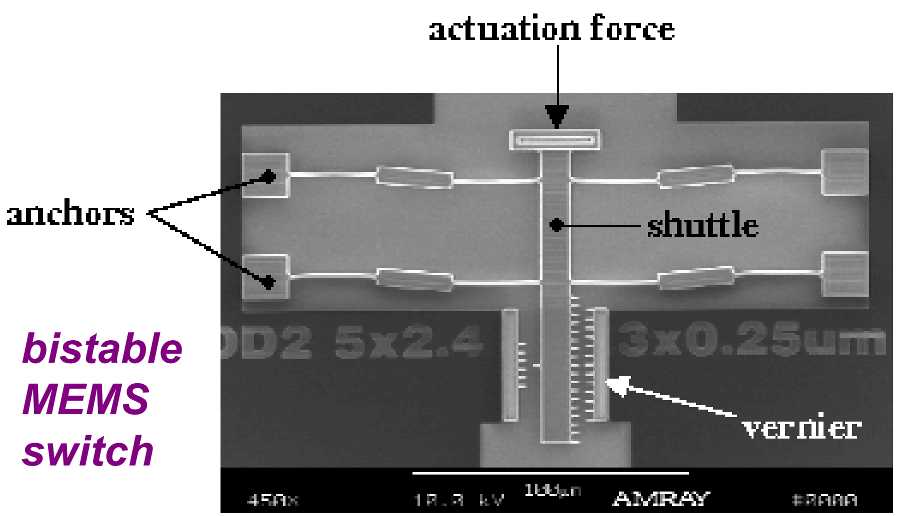
To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.

- Ubiquitous computational simulation
- Why consider uncertainty quantification (UQ)
- Propagating uncertainty through models
  - Intro to UQ methods
  - Advanced UQ methods in DAKOTA
- **Reliability-based MEMS design (OPT+UQ)**
- **Research challenges in electrical circuit UQ**



Shape Optimization of Compliant MEMS

- **Micro-electromechanical system (MEMS):** typically made from silicon, polymers, or metals; used as micro-scale sensors, actuators, switches, and machines
- **MEMS designs are subject to substantial variability** and lack historical knowledge base. Materials and micromachining, photo lithography, etching processes all yield uncertainty.
- Resulting part yields can be low or have poor cycle durability
- **Goal: shape optimize finite element model of 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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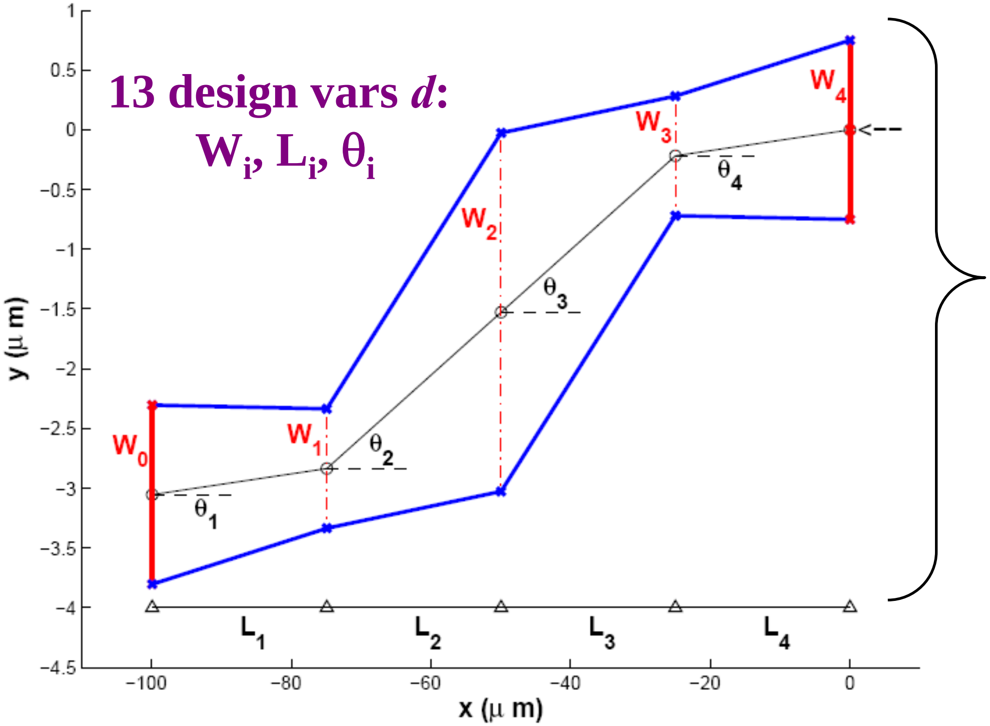
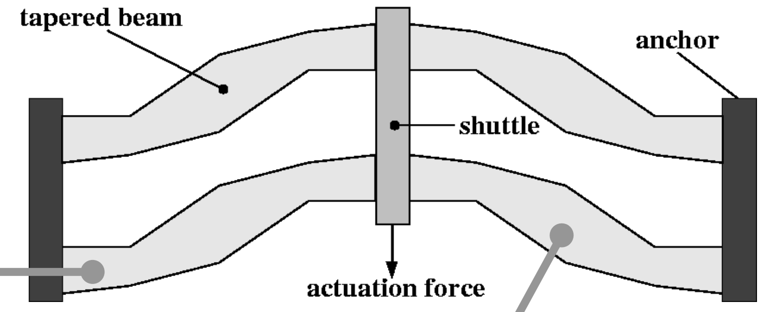
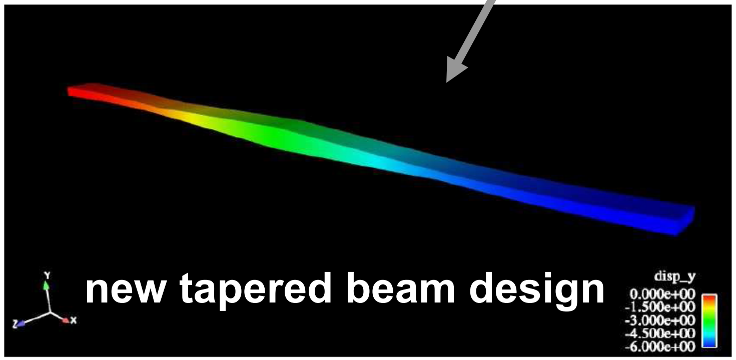
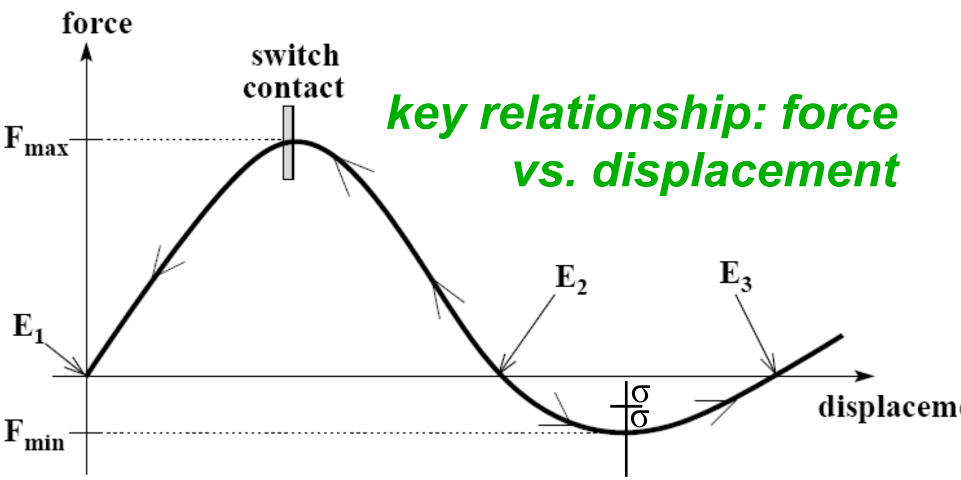
Tapered Beam Bistable Switch: Performance Metrics









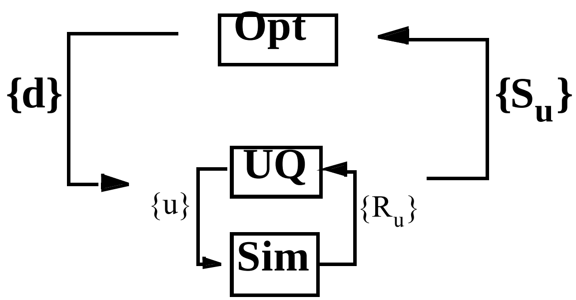
key relationship: force vs. displacement

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**

Optimization Under Uncertainty

Rather than design and then post-process to evaluate uncertainty…
actively design optimize while accounting for uncertainty/reliability metrics $s_u(d)$, e.g., mean, variance, reliability, probability:



(nested paradigm)

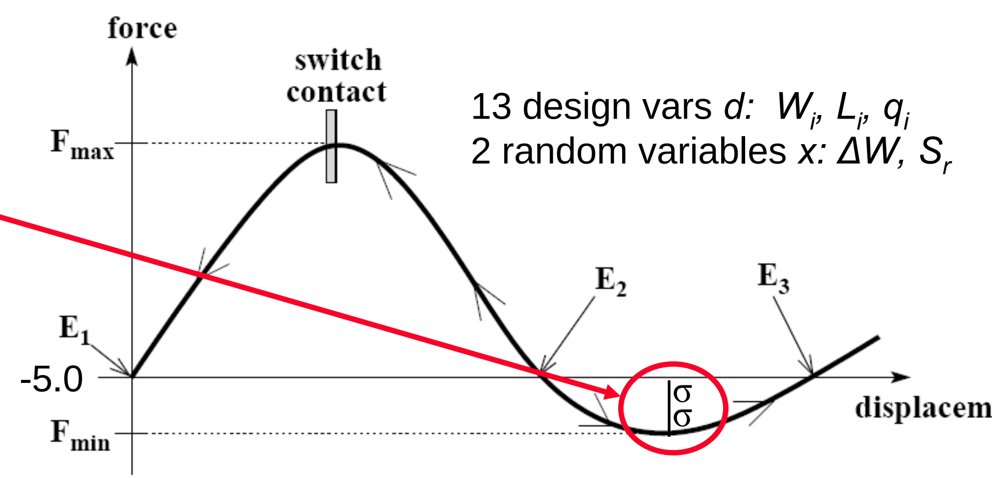
$$
\begin{aligned}
\min \quad & f(d) + W s_u(d) \\
\text{s.t.} \quad & g_l \le g(d) \le g_u \\
& h(d) = h_t \\
& d_l \le d \le d_u \\
& a_l \le A_i\, s_u(d) \le a_u \\
& A_e\, s_u(d) = a_t
\end{aligned}
$$

Bistable switch problem formulation (Reliability-Based Design Optimization):

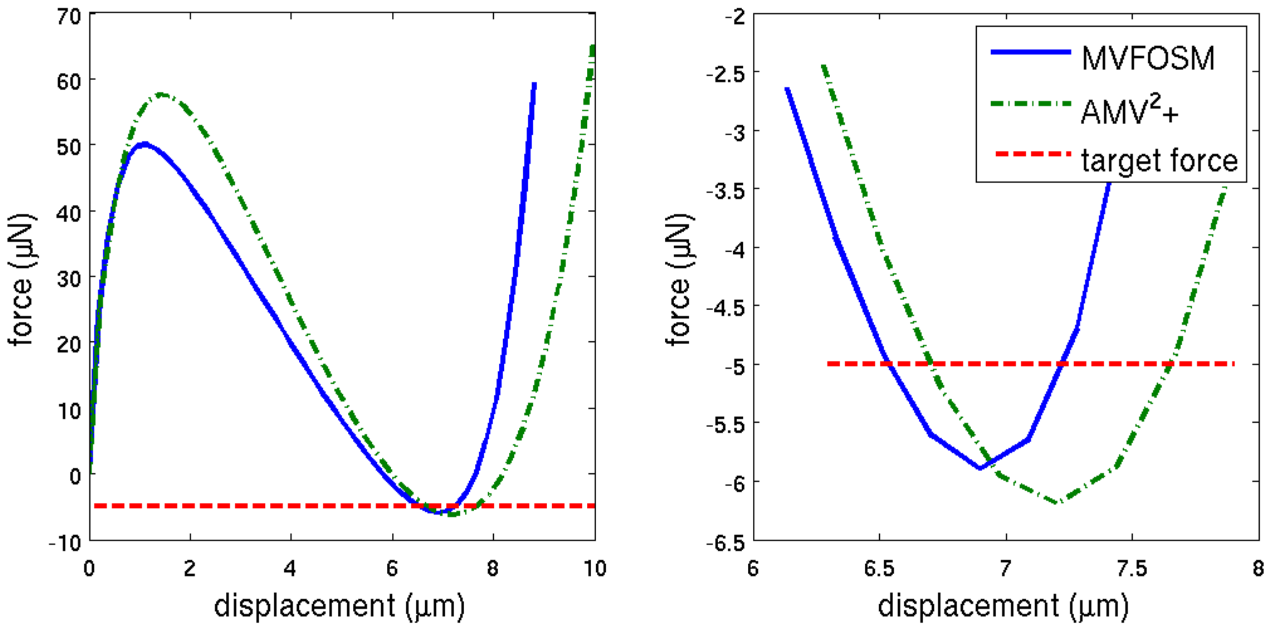
simultaneously reliable and robust designs

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

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



RBDO Finds Optimal & Robust Design



Close-coupled results: DIRECT / CONMIN + reliability method yield optimal and reliable/robust design:

metric				MVFOSM	AMV^2+	FORM
l.b.	name	u.b.	initial $\mathbf{d}^0$	optimal $\mathbf{d}^*_M$	optimal $\mathbf{d}^*_A$	optimal $\mathbf{d}^*_F$
	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	-

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DAKOTA UQ Algorithms Summary
Goal: bridge robustness/efficiency gap

	Production	New	Under dev.	Planned	Collabs.
Sampling	LHS/MC, QMC/CVT	IS/AIS/MMAIS, Incremental LHS		Bootstrap, Jackknife	Gunzburger
Reliability	$1^{st}/2^{nd}$-order local: MVFOSM/SOSM, x/u AMV/AMV^2/ AMV+/AMV^2+, x/u TANA, FORM/SORM	Global: EGRA			Renaud, Mahadevan
Polynomial chaos/ Stochastic collocation		Wiener-Askey gPC: sampling, quad/cubature, pt collocation SC: quadrature	SC: cubature gPC/SC: arbitrary input PDFs	Adaptivity, Wiener-Haar	Ghanem
Other probabilistic				Dimension reduction	Youn
Epistemic	Second-order probability	Dempster-Shafer evidence theory		Bayesian, Imprecise probability	Higdon, Williams, Ferson
Metrics	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		Storlie

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- Reliability-based MEMS design (OPT+UQ)
- **Research challenges in electrical circuit UQ**

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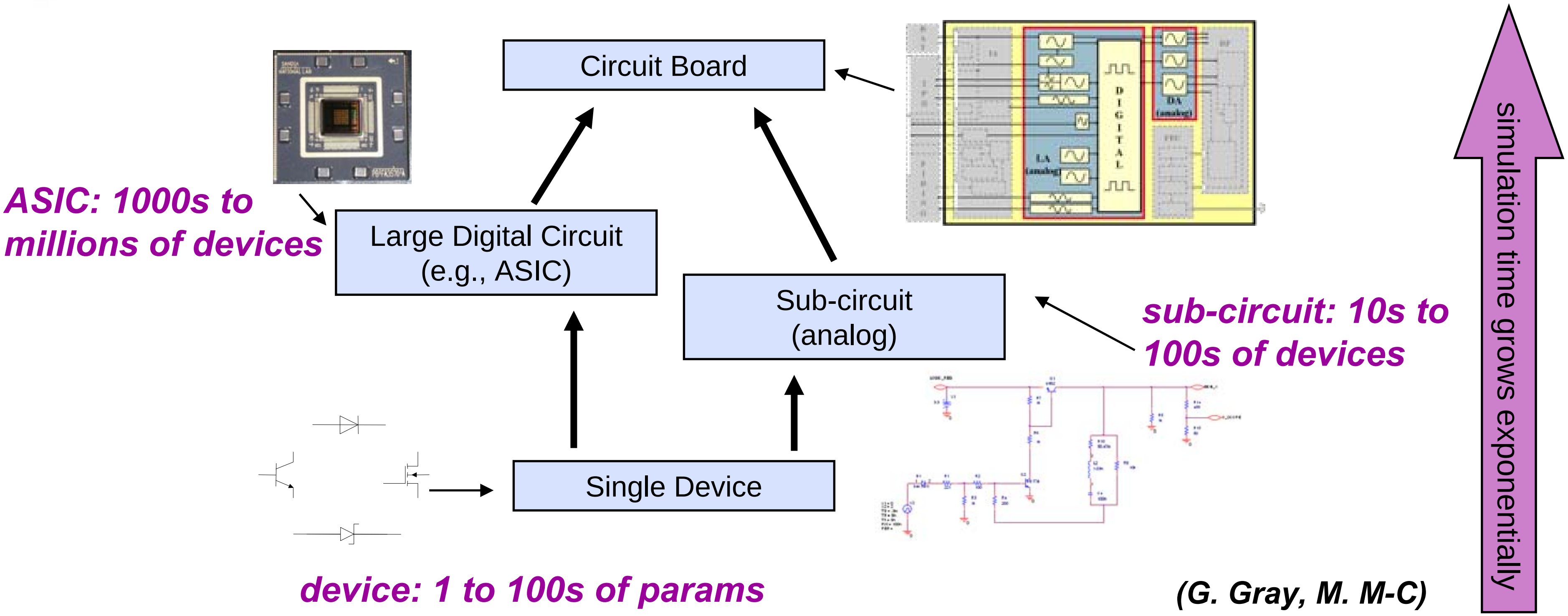
Electrical Modeling Complexity



- **simple devices:** 1 parameter, typically physical and measurable
- e.g., resistor @ 100Ω +/- 1%
- resistors, capacitors, inductors, voltage sources

- **complex devices:** many parameters, some physical, others "extracted" (calibrated)
- multiple modes of operation
- e.g., zener diode: 30 parameters, 3 bias states; many transistor models (forward, reverse, breakdown modes)

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Electrical Circuit UQ

- **Circuit analysis challenges**
  - network of nonlinearly coupled components, feedback loops, staged behavior, or discrete digital logic, mandating all-at-once circuit solution techniques
  - long simulation time involving iterative solvers (often hours to simulate microseconds, particularly in oscillating electronics);
  - combination of analog and digital circuits: consider separately or together
    - analog circuits typically < 100 devices, including replicates, less predictable topology across designs
    - digital circuits 1,000 to 1,000,000 transistors (identical or similar), small number of well-defined connection types.

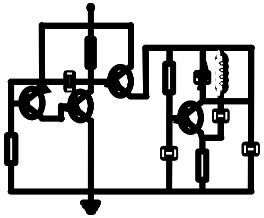
- **Typical parametric uncertainties**:
  - process parameters (e.g., diffusion times, oven temperatures)
  - physical parameters (e.g., line widths, channel doping)
  - model parameters (e.g., BSIM3 transistor compact model)
  - electrical parameters (e.g., line resistance, saturation current, threshold voltage)
- Mapping reality to compact model parameters not always easy; compact model may be more behavioral than physics-based

UQ: Explosion of Factors!

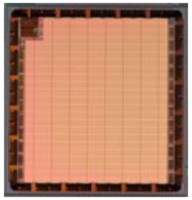
complex device models + replicates in circuits

- **Tor Fjeldy radiation photocurrent models for transistors**
  - **20 model parameters, three levels for each (low, nominal, high) ~ 3 billion combinations**
  - **not practical via factorial brute force, but LHS might miss extreme "corner" behaviors**
  - **6 devices in circuit of interest; mitigated via OAs**

- **Simple voltage regulator circuit**
  - **4 BJTs, 1 MOSFET, 17 resistors, 1 capacitor, 1 zener diode**
  - **over 100 parameters if considered naively**
  - **mitigate by determining parameter sets giving rise to low, nominal, high response for each device**



- **CMOS 7 ViArray: generic ASIC implementation platform**
  - **Approx 1 million transistors**
  - **adding parasitics yields a simulation with millions of resistors, capacitors, inductors**
  - **mitigated by grouping within process layers**



Approaches curbing the curse of dimensionality crucial in analyzing these kinds of systems!

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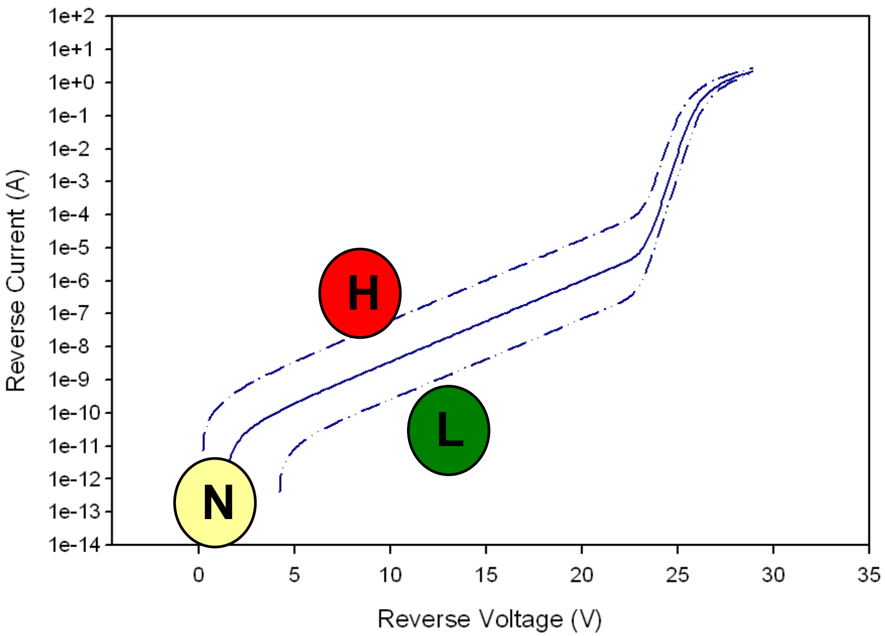
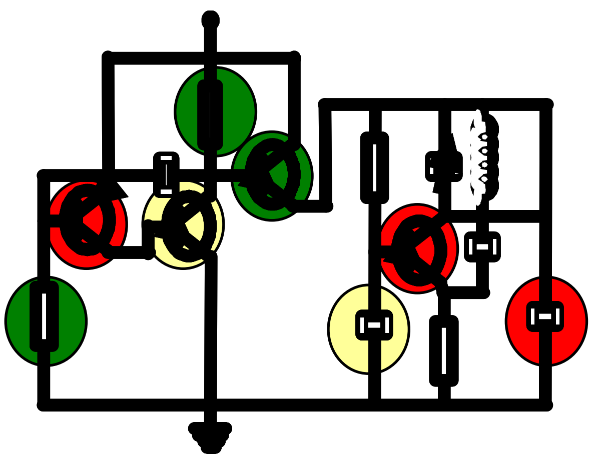
Zener Low-Nominal-High Models

- For single device, perform LHS samples of 20 parameters
- Determine 3 sets of parameters giving rise to nominal and extreme device response
- When performing circuit UQ, sample uniformly from L,N,H and set all 20 parameters accordingly in the full simulation





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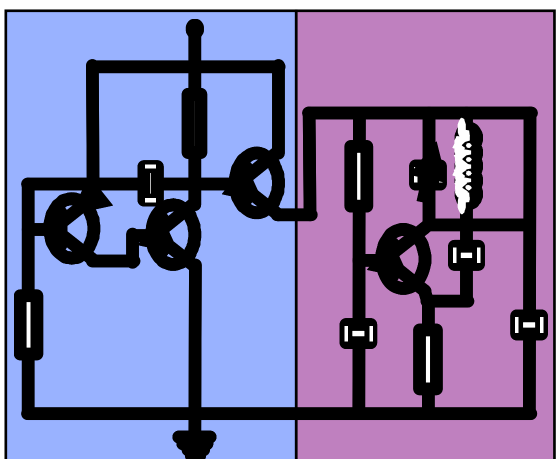
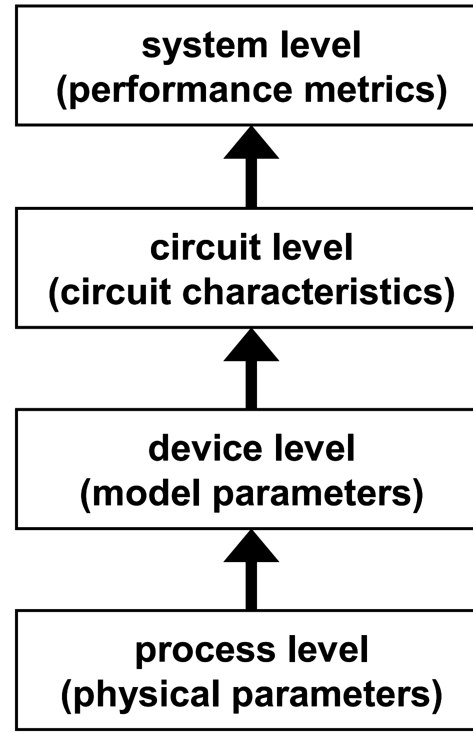
Hierarchical/Network Structure

- How can we exploit electrical systems' natural hierarchy or network structure?
- How does uncertainty propagate? Sufficient to propagate variance?
- Use surrogate/macro-models as glue between levels?
- Can approaches be implemented generically to apply to any circuit implemented in Xyce?





Other Relevant Technologies

- Apply existing reliability and polynomial chaos methods; benefit of embedded techniques?

- Principal components analysis (PCA, SVD, POD), reduced-order modeling techniques: only vary uncorrelated parameters

- Surrogate/macro modeling, insert current/voltage sources representative of the effect of uncertainty

- Leverage structure of network, DAE system under the hood; automatic structure analysis, macro-model creation?

Summary

To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.

- **Uncertainty quantification algorithms are essential in credible simulation**
- **Complex, large-scale simulations demand research in advanced efficient UQ methods**

Thank you for your attention!

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Abstract

- 2008 CSRI Summer Lecture Series
- Title: "From uncertainty to credibility: UQ algorithms and research challenges"
- Speaker: Brian Adams (Org. 1411)
- Date/Time: Wednesday, July 2, 3-4pm (MST)
- Location:
- NM: CSRI/90
- CA: 915/S145
- Abstract:

- Computational simulations are routinely used to assess the performance, reliability, and safety of existing and proposed systems, and are increasingly used for risk-informed decision making in the presence of uncertainties. To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.
- Uncertainty quantification (UQ) algorithms compute the effect of uncertain input variables on response metrics of interest, enabling risk assessment, model calibration, and model validation. In this talk, I will motivate simulation-based UQ with examples from electrical circuit and MEMS design. I will survey methods from ubiquitous Monte Carlo sampling through more advanced reliability analysis and polynomial chaos expansions available in Sandia's DAKOTA toolkit. In particular, DAKOTA's reliability analysis methods employ a mix of probability, optimization, and surrogate (meta-) modeling to efficiently perform UQ.
- Challenges in large-scale electrical circuit UQ will motivate unmet algorithm research needs.

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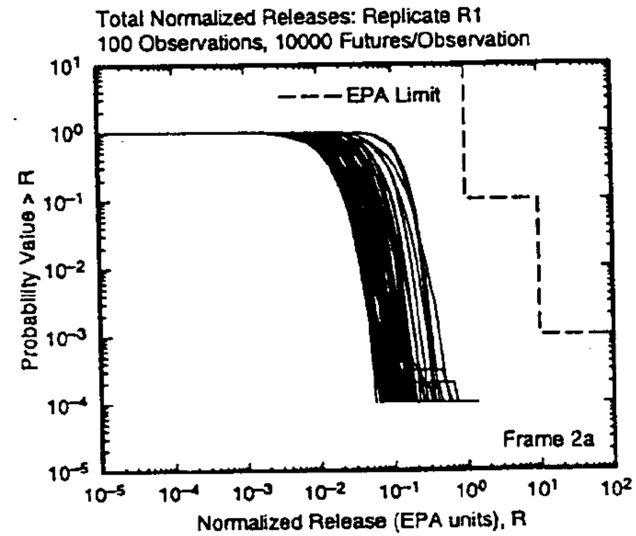
Extra Slides

Epistemic UQ

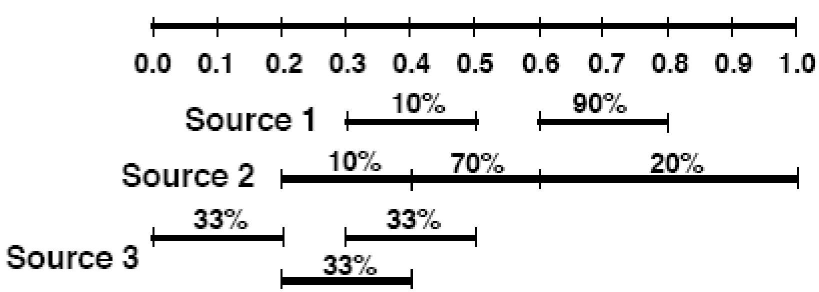
Second-order probability

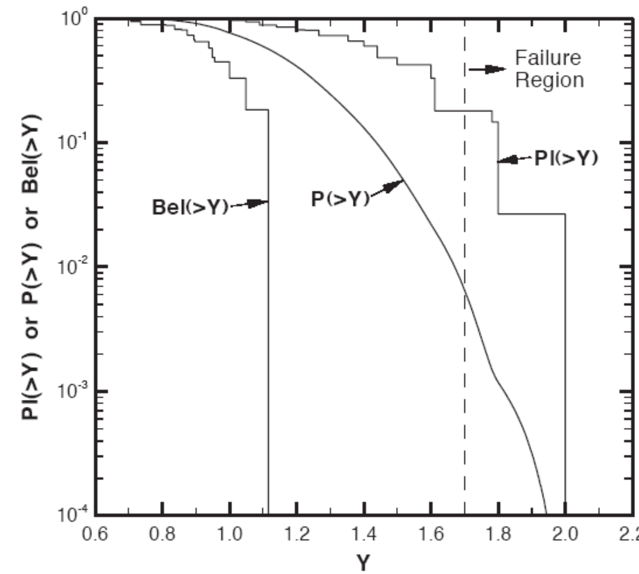
- Two levels: distributions/intervals on distribution parameters
- New — Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).



Dempster-Shafer theory of evidence

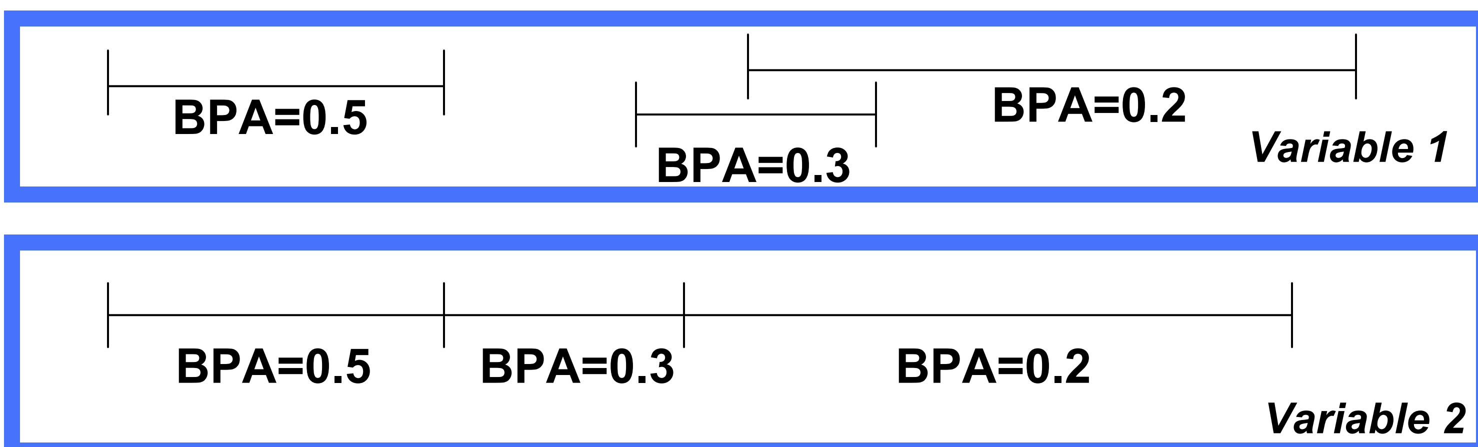
- Basic probability assignment (interval-based)
- New — Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals





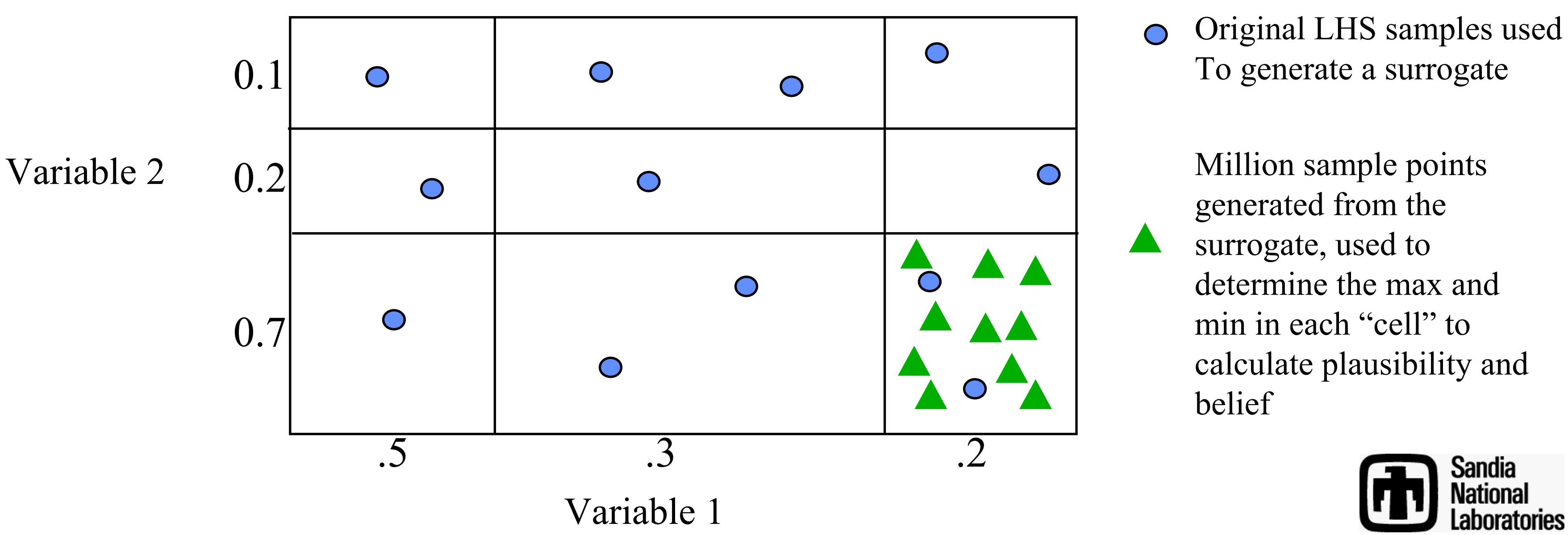
Epistemic Uncertainty Quantification

- 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



Bayesian Analysis

- Construct a prior distribution on a parameter (which might be a parameter of a distribution)
- The prior distribution should be based on previous experience, engineering judgment
- The distribution on the prior is updated with actual data. The resulting updated distribution is called the posterior.

Frequentist	Bayesian
Assumes there is an unknown but fixed parameter θ	Assumes a distribution on unknown parameter θ
Estimates θ with some confidence interval	Uses probability theory, treats θ as a random variable

Bayesian Analysis

- Why would we use it for CS&E problems?
- Nice feature of incorporating additional data as it becomes available
- We often don't have good estimates: Bayes provides a framework for starting with what we do know, and refining our estimates in a statistically consistent manner
- Examples:
  - Reliability problems: Update probability of failure
  - Response surfaces: Update parameters in a surrogate model for a trust region
  - Calibration under Uncertainty (CUU): Update our parameter estimates based on experimental data AND uncertainty in a model

Bayesian Methods

Discrete Case

$$p(\theta \mid \mathbf{x}) = \frac{p(\mathbf{x},\theta)}{p(\mathbf{x})} = \frac{p(\mathbf{x} \mid \theta)\, p(\theta)}{p(\mathbf{x})} = \frac{p(\mathbf{x} \mid \theta)\, p(\theta)}{\sum_{\theta} p(\mathbf{x} \mid \theta)\, p(\theta)}$$

where θ is a parameter(s), x is a data vector, and p is a probability mass function.

$$p(\theta \mid \mathbf{x}) = posterior \propto p(\mathbf{x} \mid \theta)\, p(\theta) = likelihood * prior$$

Examples

- **Use Binomial distribution to model the number of failures, x, in n trials.**

$$f(x \mid \theta) = \binom{n}{x} \theta^x (1-\theta)^{n-x}$$

- **We obtain data that shows 2 failures in 5 trials**

Prior Probability	Posterior Probability
P{θ=0.3}=0.1	P{θ=0.3}=0.13
P{θ=0.6}=0.9	P{θ=0.6}=0.87

- **The posterior distribution reflects the fact that in this set of data, θ = 0.4 which is closer to 0.3 than 0.6 and so the probability of θ=0.3 has risen slightly.**

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