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Advanced Uncertainty Quantification for Optimization under Uncertainty

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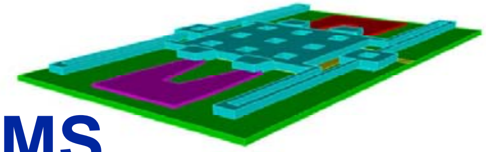
Outline

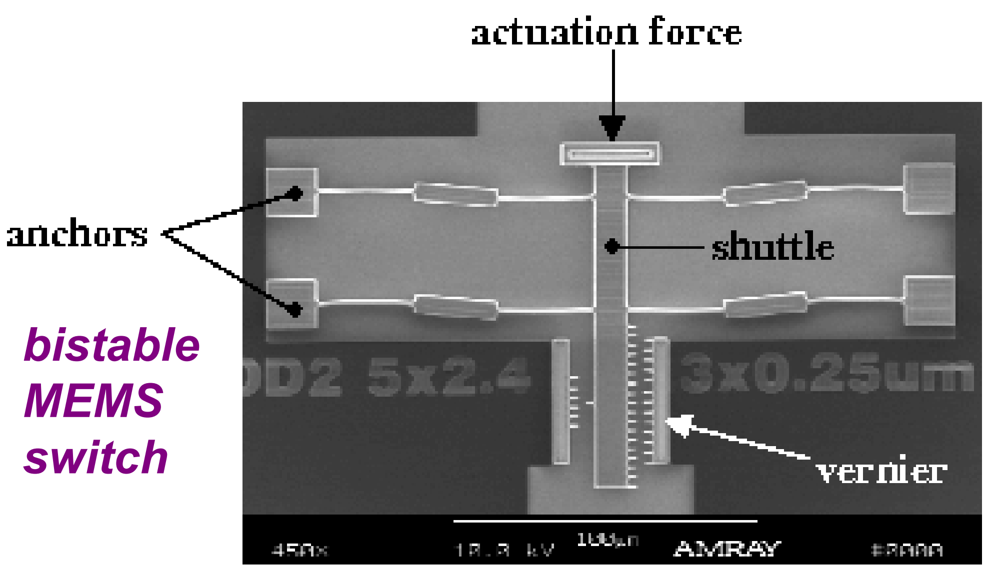
Focus: simulation-based optimization with efficient in-the-loop quantification of parametric uncertainty

- **Motivation: design optimization of MEMS bistable switch**
- **Survey of uncertainty quantification algorithms for assessing parametric uncertainty**
- **DAKOTA framework: integrating optimization and uncertainty quantification**
- **Design under uncertainty for MEMS**



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)

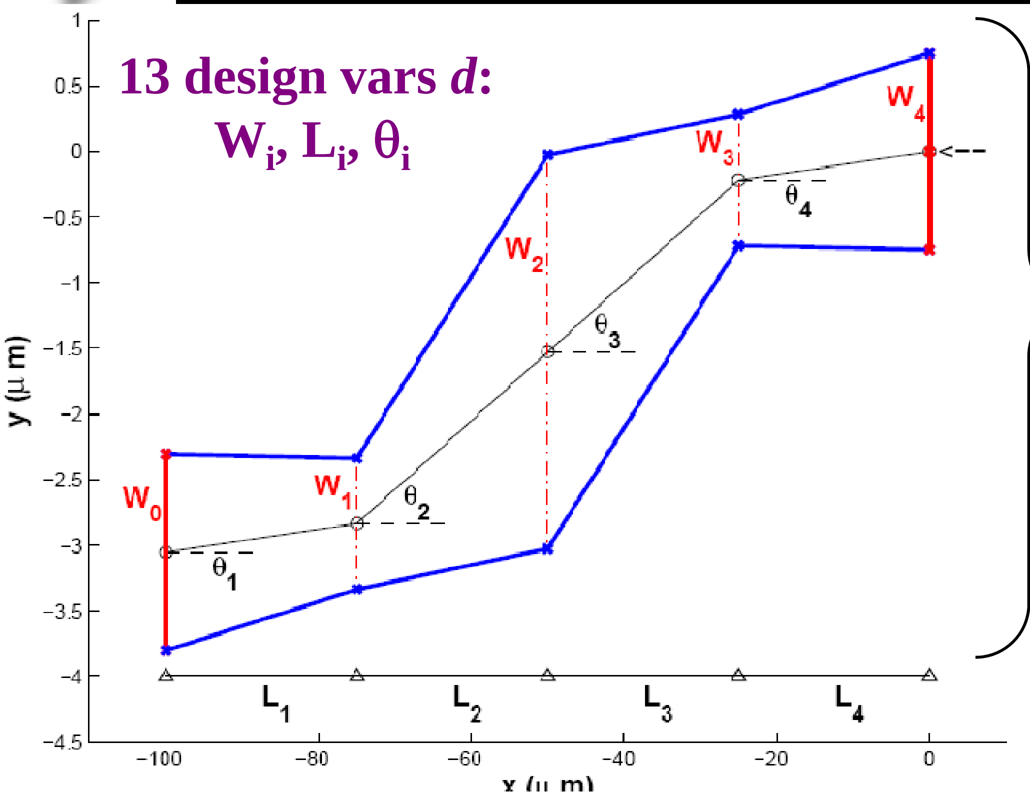


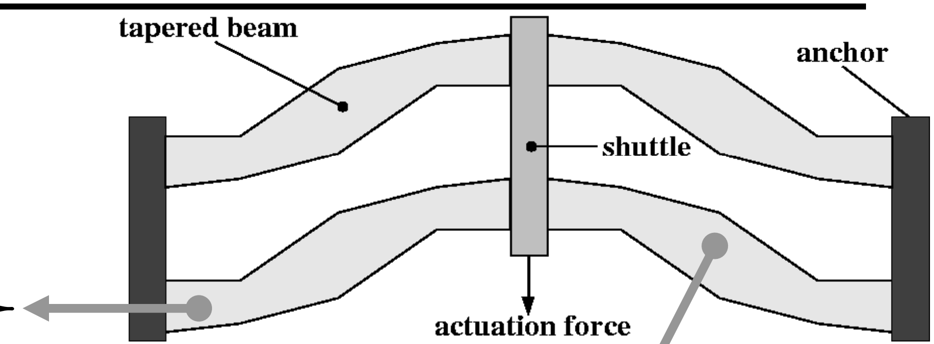
bistable MEMS switch

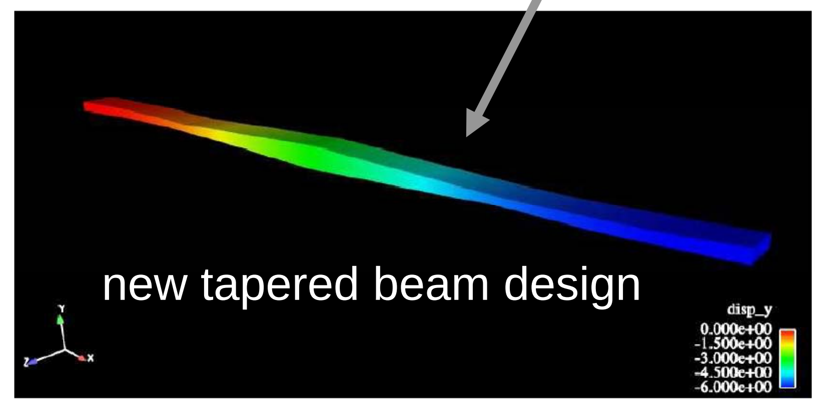
uncertainties to be considered (edge bias and residual stress)

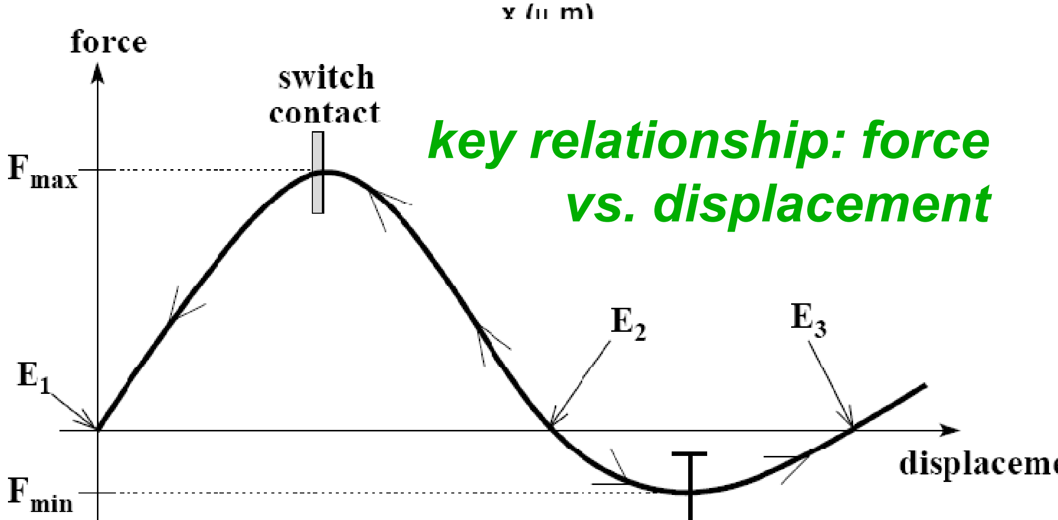
variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

Tapered Beam Bistable MEMS 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**

Uncertainties in Simulation and Validation

A single optimal design or nominal performance prediction is insufficient; a *few* uncertainties affecting computational models:

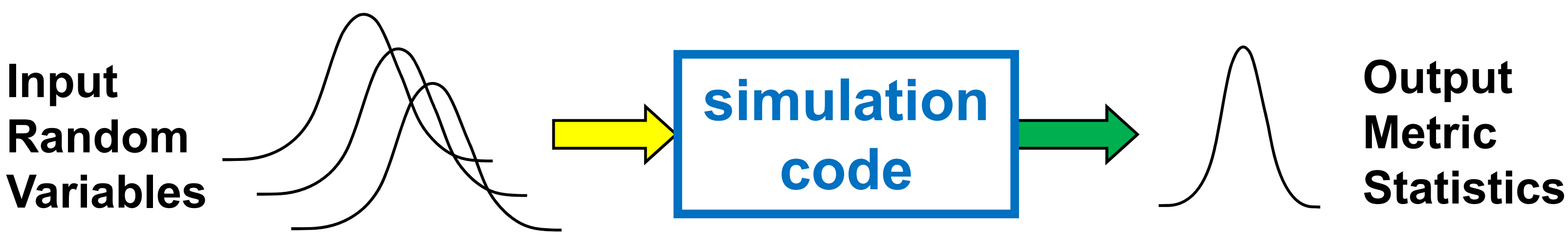
- physics/science parameters
- statistical variation, inherent randomness
- model form / accuracy
- operating environment, interference
- initial, boundary conditions; forcing
- geometry / structure / connectivity
- material properties
- manufacturing quality
- experimental error (measurement error,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

The effect of these on model outputs should be integral to an analyst's deliverable: *best estimate PLUS uncertainty!*

Characterizations of Uncertainty

Often useful algorithmic distinctions, but not always a clear division

- **Aleatory** ***(think probability density function; sufficient data)***
  - **Inherent variability (e.g., in a population), type-A, stochastic**
  - **Irreducible uncertainty – can't reduce it by further knowledge**



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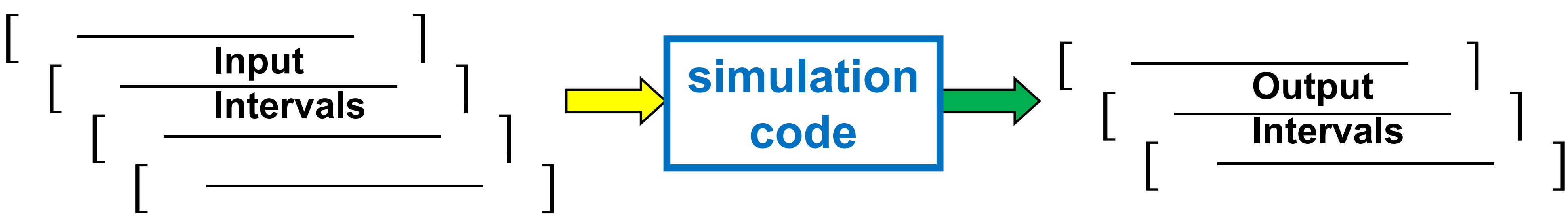
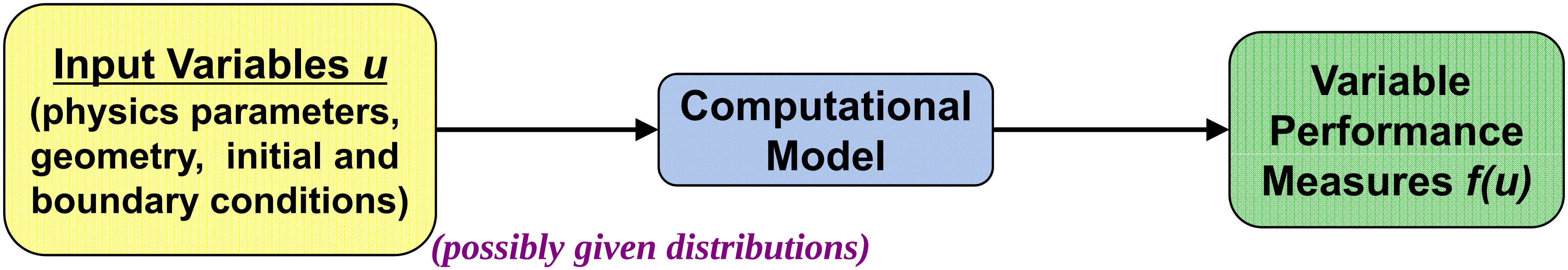
  - **Irreducible uncertainty – can't reduce it by further knowledge**

- **Epistemic** ***(think bounded intervals)***
  - **Subjective, type-B, state of knowledge 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**



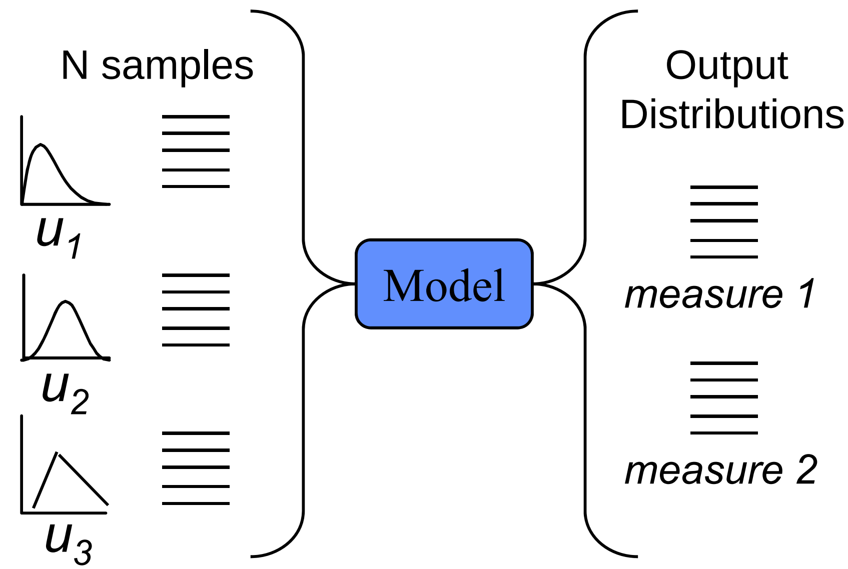
Uncertainty Quantification

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



Potential Goals:

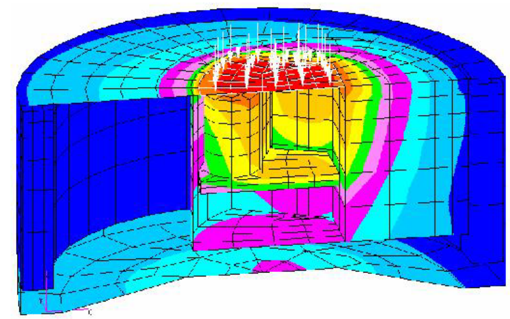
- **based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)**
- **risk-informed/uncertainty-aware decision making / trade-off assessment**
- **quantification of margins and uncertainties (QMU)**
- ***assess how close uncertainty-aware code predictions are to data, required performance, or crucial limits***

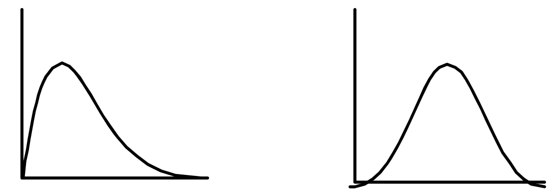


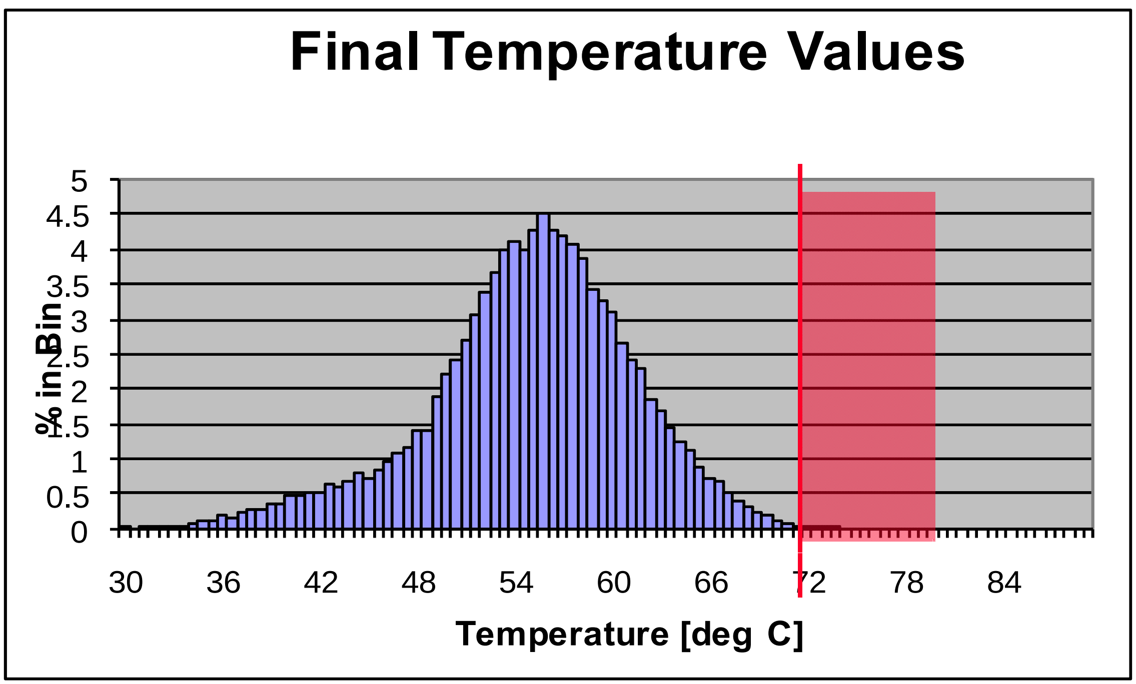
Typical method: Monte Carlo sampling

Example: Thermal Uncertainty Quantification

- **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:

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

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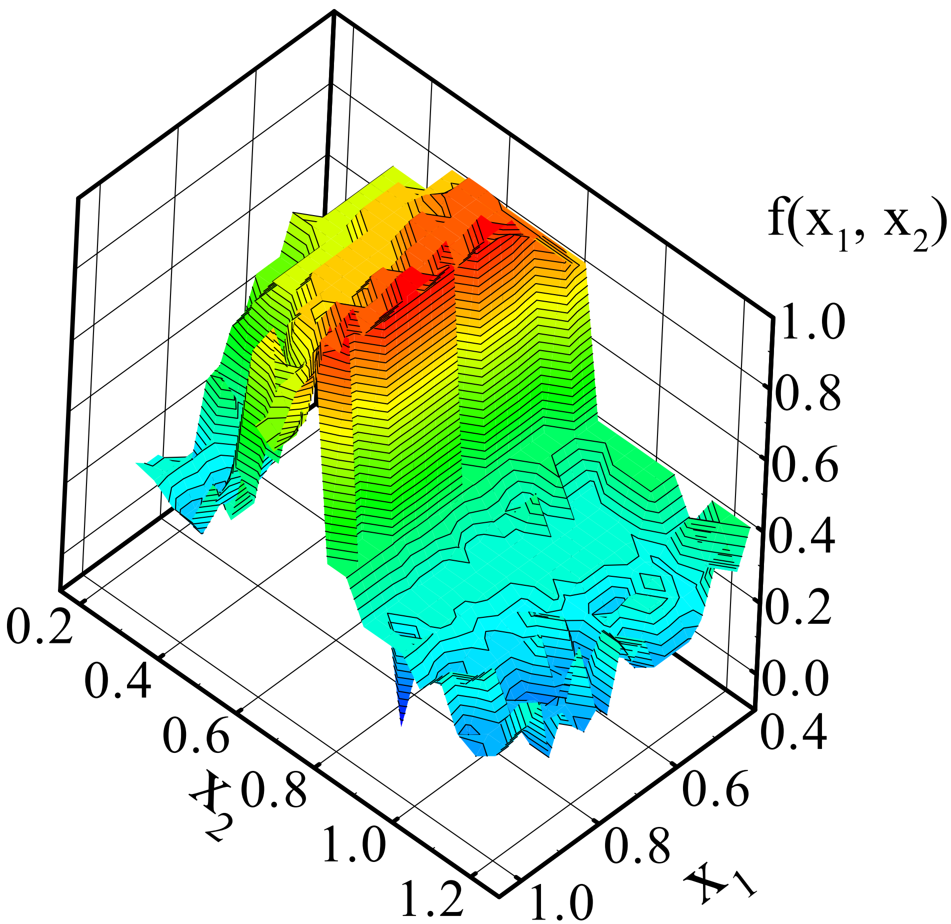
Challenges for Simulation-based UQ

- **Similar to optimization for a simulation-based engineering application, but propagate uncertainty through computer model.**
- **Need statistics of response function *f*, e.g., μ_f, σ_f, Prob[$f > f_{critical}$]**
- **Typical characteristics:**



- **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**

DAKOTA toolkit attempts to mitigate these issues; *a mix of statistics, nonlinear optimization, numerical integration, and surrogate (meta-) modeling enables robust and efficient UQ methods.*

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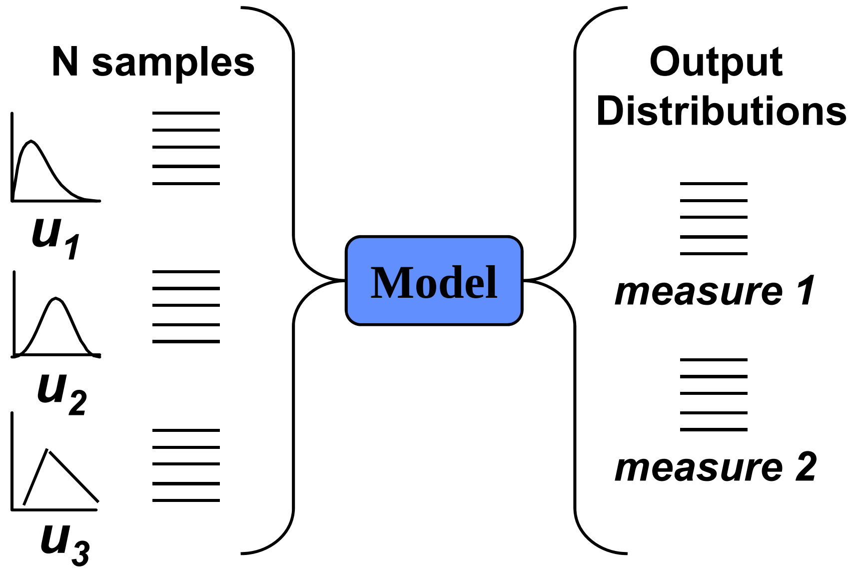
UQ: Sampling Methods

Given distributions of $u_1,\ldots,u_N$, sampling-based methods calculate sample statistics, e.g., on temperature $T(u_1,\ldots,u_N)$:



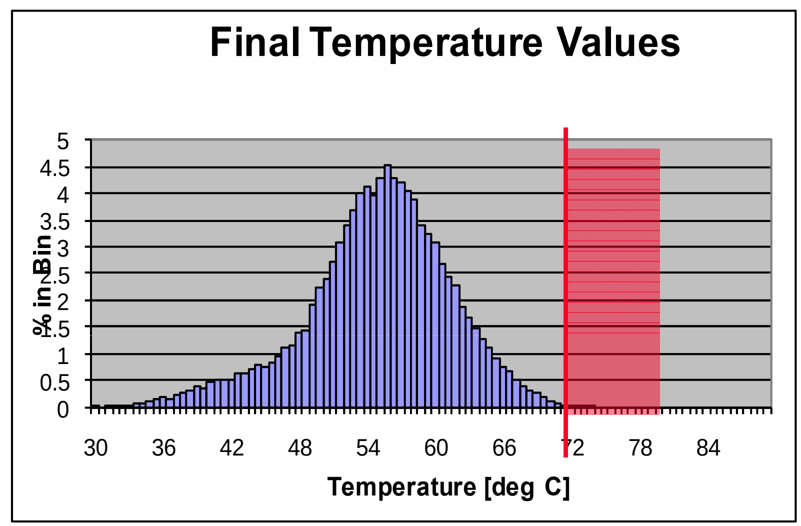
- **sample mean**

$$\overline{T} = \frac{1}{N}\sum_{i=1}^{N} T(u^i)$$

- **sample variance**

$$T_{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}\left[T(u^i) - \overline{T}\right]^2$$

- **full PDF(probabilities)**

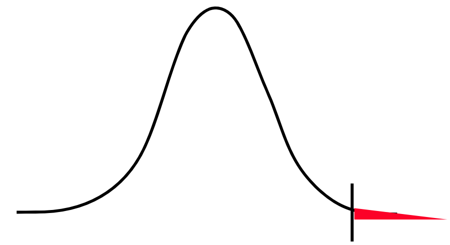


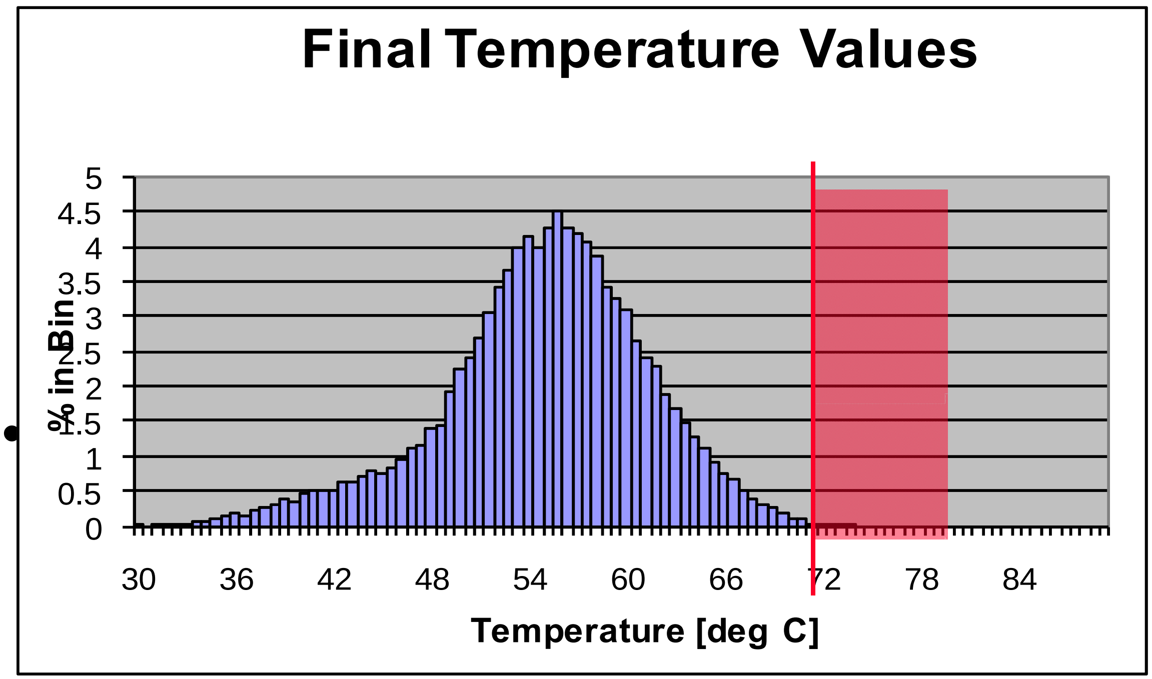
- **Monte Carlo sampling**
- **Quasi-Monte Carlo**
- **Centroidal Voroni Tessalation (CVT)**
- **Latin Hypercube sampling**

Robust, but slow convergence: $O(N^{-1/2})$

Calculating Probability of Failure

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





- **Could perform 10,000 LHS samples and count how many exceed threshold…**
- **…or MV: make a linearity (and possibly normality) assumption and project…**
- **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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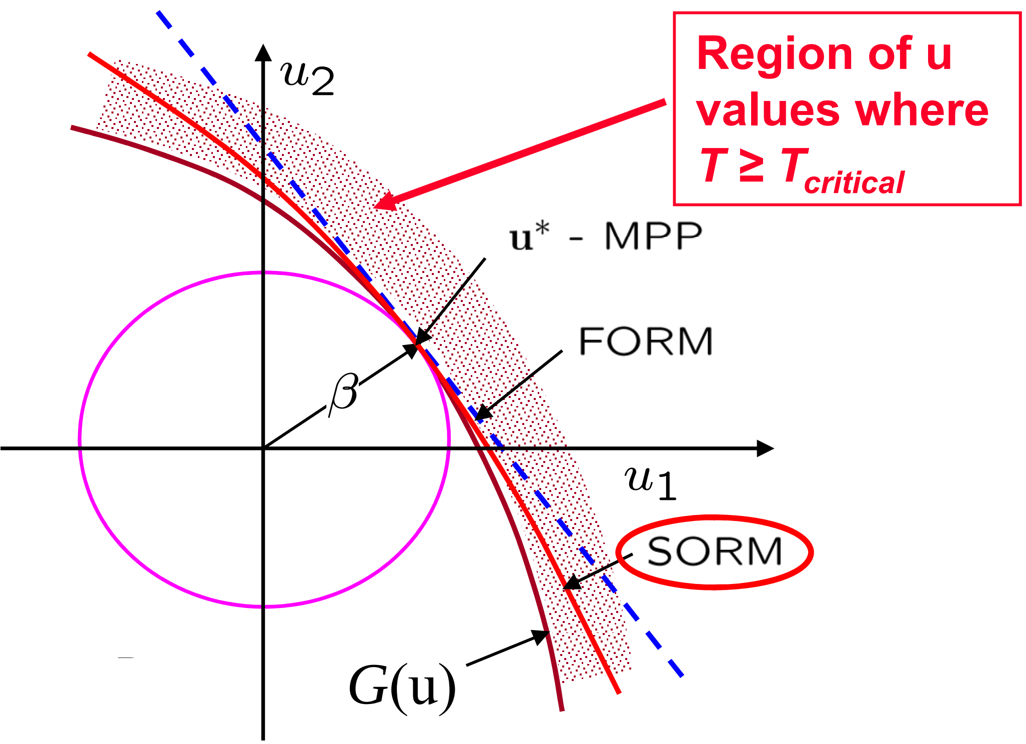
Analytic Reliability: MPP Search

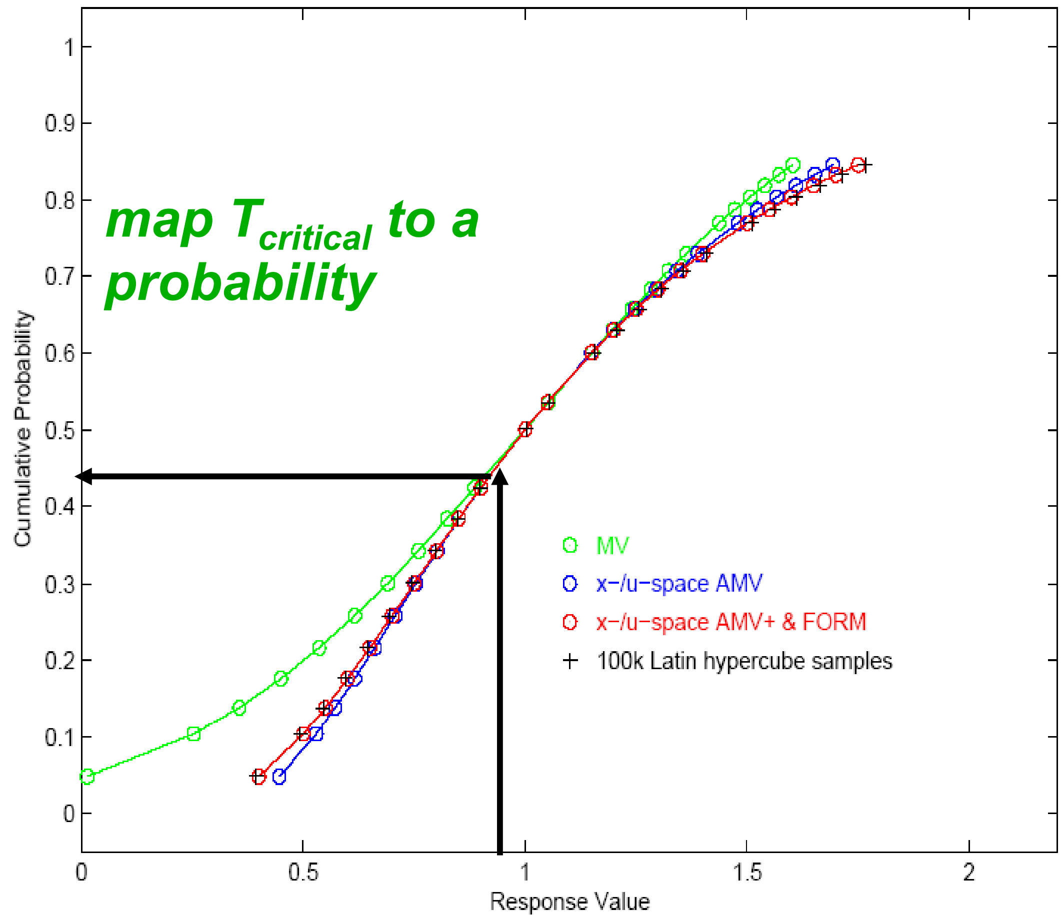
Perform optimization **in uncertain variable space to determine Most Probable Point (of response or failure occurring) for *G(u)* = *T(u)*.**

Reliability Index Approach (RIA)

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



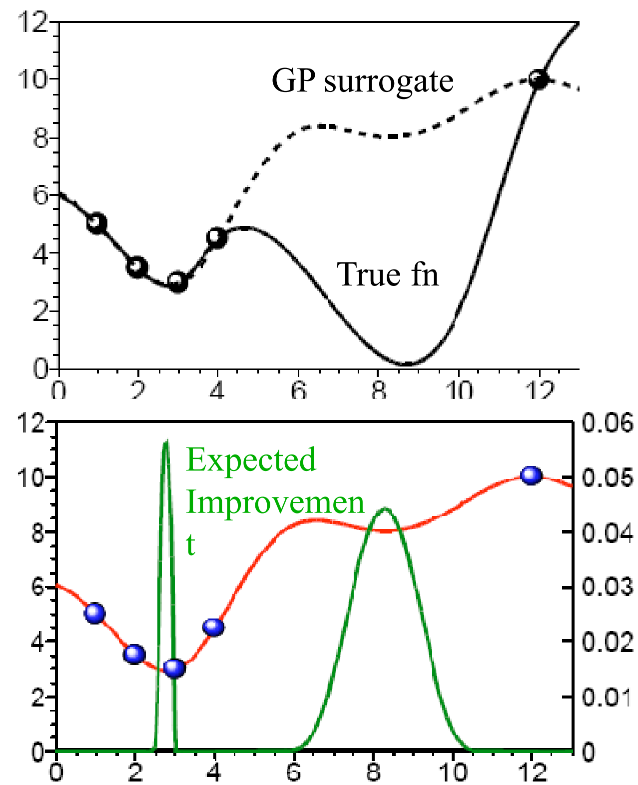
analytic derivatives of statistics w.r.t. design variables



Efficient Global Reliability Analysis

- **EGRA** (B.J. Bichon) performs reliability analysis with
  - EGO Gaussian Process surrogate with NCSU DIRECT optimizer
  - multimodal adaptive importance sampling for probability calculation
- Created to address nonlinear and/or multi-modal limit states in MPP searches.

- In efficient global optimization (EGO): expected improvement is large near promising minima, or in regions of high uncertainty



From Jones, Schonlau, Welch, 1998

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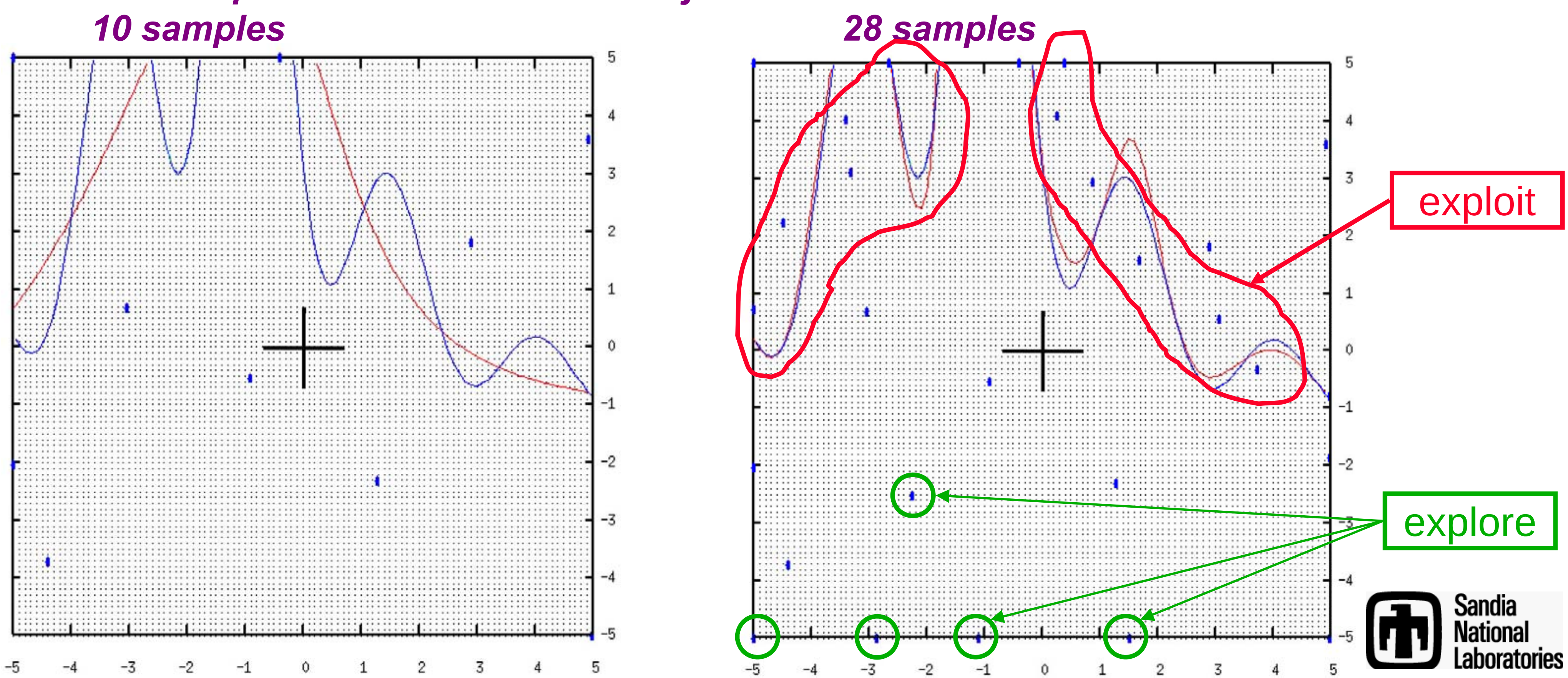
Efficient Global Reliability Analysis

- Apply an EGO-like method to the equality-constrained optimization problem
- In EGRA, an expected feasibility function balances exploration with local search near the failure boundary to refine the GP
- Cost competitive with best MPP search methods, yet better probability of failure estimates

Gaussian process model of reliability limit state with



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Stochastic Expansions

- **Create global polynomial approximation to response function**
- **Polynomial chaos expansions (PCE): known basis, compute coefficients**

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

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R\, \Psi_j\, \varrho(\boldsymbol{\xi})\, d\boldsymbol{\xi}$$

- **(Lagrange) Stochastic collocation (SC): known coefficients, form interpolant**

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

- **Form basis, then sample, calculate moments, probabilities, etc.**
- **Tailoring → fine-grained algorithmic control:**
  - **Synchronize PCE form with numerical integration**
  - **Optimal basis & Gauss pts/wts for arbitrary input PDFs**
  - **Anisotropic approaches: emphasize key dimensions**
- **h/p-adaptive collocation (FY10-12)**

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Generalized Polynomial Chaos Expansions (PCE)

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**

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

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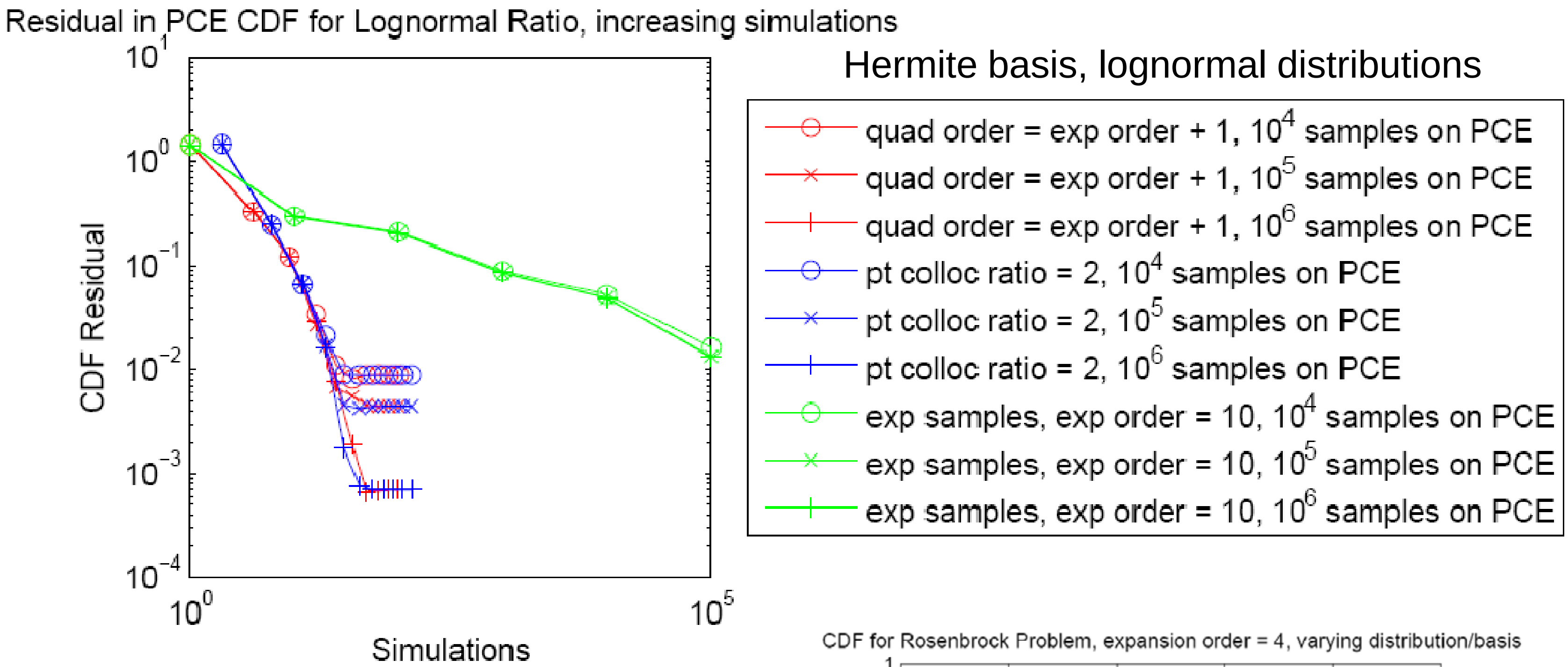
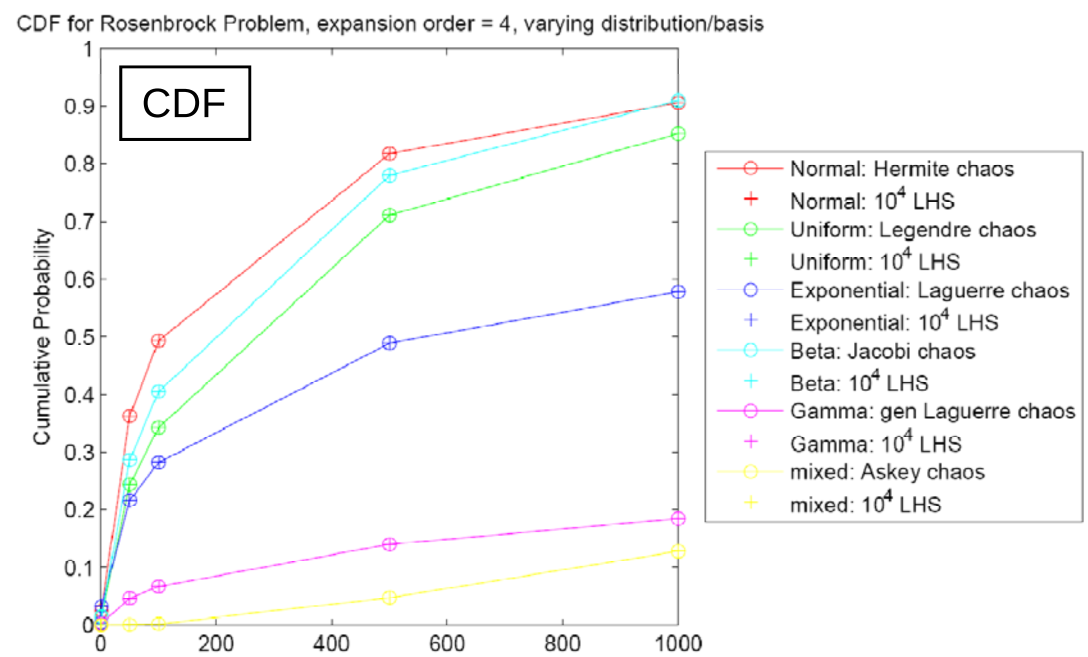
Optimal Basis + Effective Integration = Fast Convergence



also analytic derivatives of statistics w.r.t. design variables



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Uncertainty-Aware Design

Rather than designing and then post-processing to evaluate uncertainty…

Standard NLP

$$
\begin{aligned}
\text{minimize} \quad & f(d) \\
\text{subject to} \quad & g_l \le g(d) \le g_u \\
& h(d) = h_t \\
& d_l \le d \le d_u
\end{aligned}
$$

…actively design while accounting for uncertainty/reliability metrics

*Augment with general response statistics **s_u** (e.g. μ, σ, or reliability **z/β/p**) with linear map*

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

Focus on large-scale simulation-based engineering applications:

- **mostly PDE-based, often transient, some agent-based/discrete event**
- **response mappings (fns. and constraints) are nonlinear and implicit**
- **CRUCIAL: efficient means to compute statistics $s_u(d)$!**

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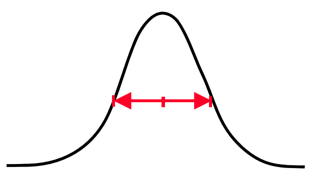
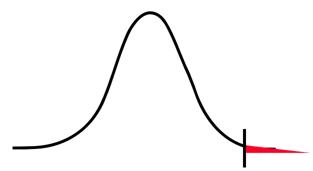
Potential Optimization under Uncertainty Goals

Design for…

…robustness:
min/constrain μ, σ², moments or G(β) range



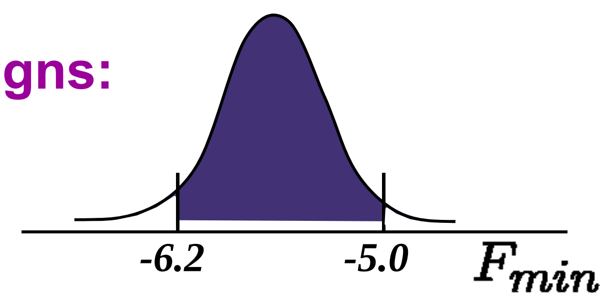
…reliability:
max/constrain *p*/β (minimize tail stats, failure)



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

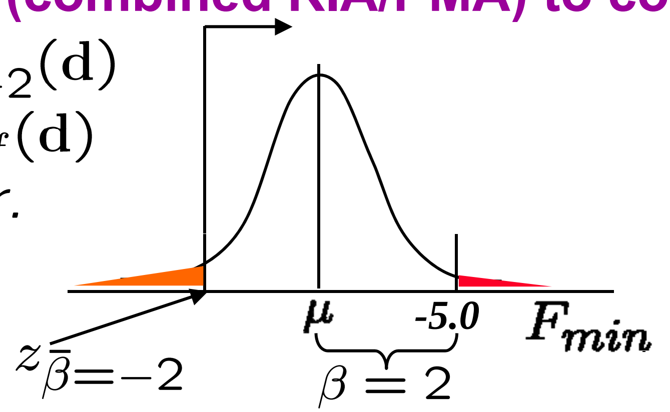
…probability s.t. limits; robust designs:

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



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

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



(DAKOTA flexibly allows RIA/PMA combinations)

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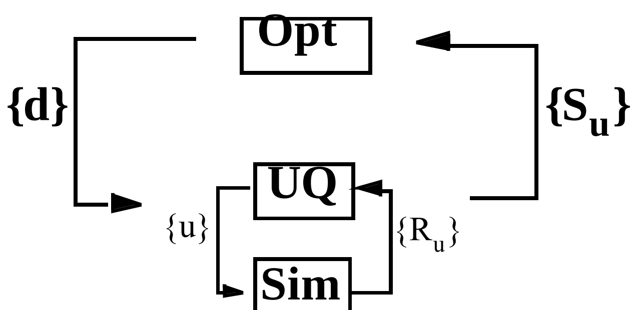
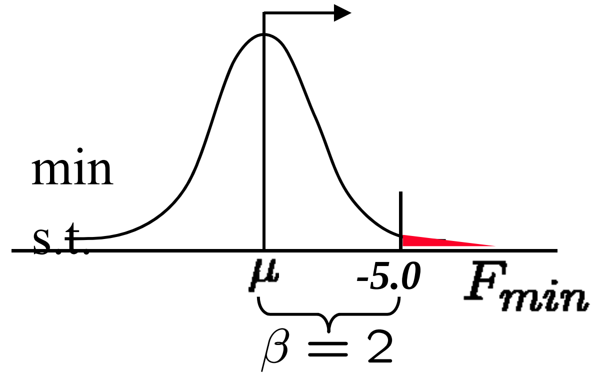
Optimization Under Uncertainty

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; use any UQ algorithm

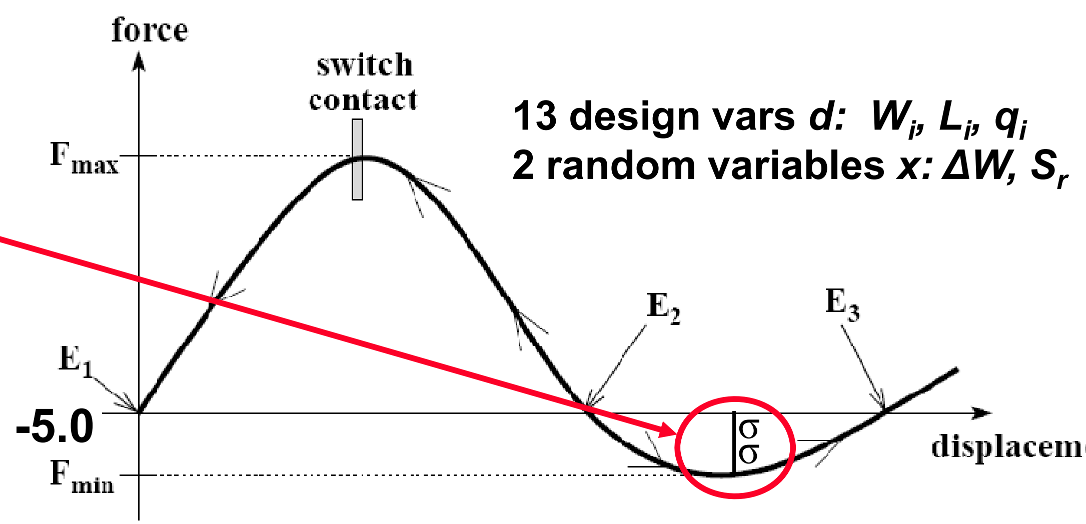
$$\begin{aligned} \min \quad & f(d) + W\, s_u(d) \\ \text{s.t.} \quad & g_l \leq g(d) \leq g_u \\ & h(d) = h_t \\ & d_l \leq d \leq d_u \\ & a_l \leq A_i\, s_u(d) \leq a_u \\ & A_e\, s_u(d) = a_t \end{aligned}$$



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

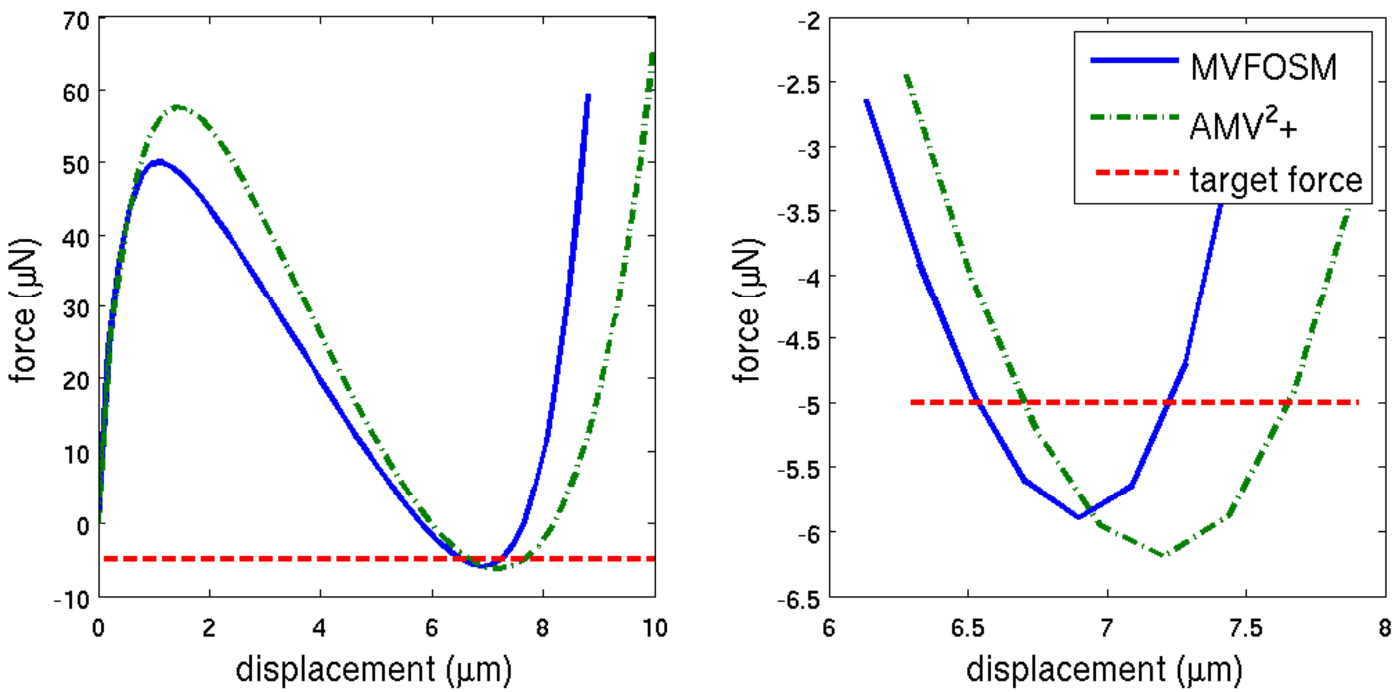
simultaneously reliable and robust designs

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



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

	Production	New	Under dev.	Planned	Collabs.
Sampling	**Latin Hypercube, Monte Carlo**	**Importance, Incremental**		**Bootstrap, Jackknife**	**FSU**
Reliability	***Local:* Mean Value, First-order & second-order reliability methods (FORM, SORM)**	***Global:* Efficient global reliability analysis (EGRA)**			***Local:* Notre Dame, *Global:* Vanderbilt**
Stochastic expansion	Adv. Deployment Fills Gaps	**Tailored polynomial chaos & stochastic collocation with extended basis selection**	**Anisotropic sparse grid, cubature, p-adaptive, multiphysics**	**h-adaptive, hp-adaptive, gradient-enhanced, discrete**	**Stanford, Purdue, CU Boulder, USC, VPISU**
Other probabilistic		**Random fields/ stochastic proc.**		**Dimension reduction**	**Cornell, Maryland**
Epistemic	**Second-order probability (nested sampling)**	**Dempster-Shafer, Opt-based interval estimation**	**Bayesian**	**Imprecise probability**	**LANL, Applied Biometrics**
Metrics & Global SA	**Importance factors, Partial correlations**	**Main effects, Variance-based decomposition**	**Stepwise regression**		**UNM**

Reseach: Tailoring & Adaptivity

Summary

- Uncertainty-aware design optimization is helpful in MEMS design where robust and/or reliable designs are essential.
- Advanced UQ algorithms may offer more refined estimates of uncertainty than sampling or mean value methods and are typically more efficient in an optimization context (and may offer analytic derivatives).
- The publicly available 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.

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