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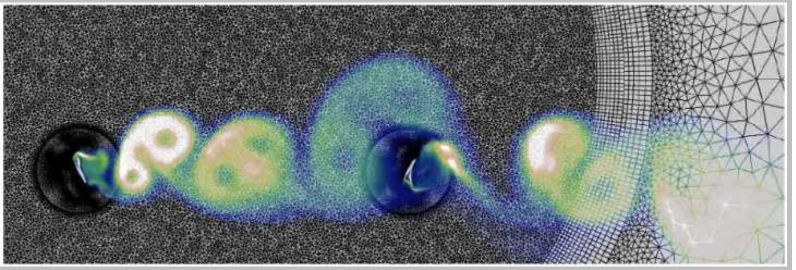

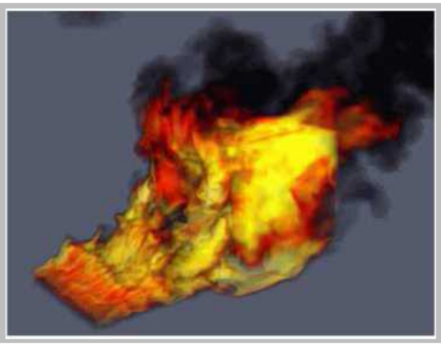

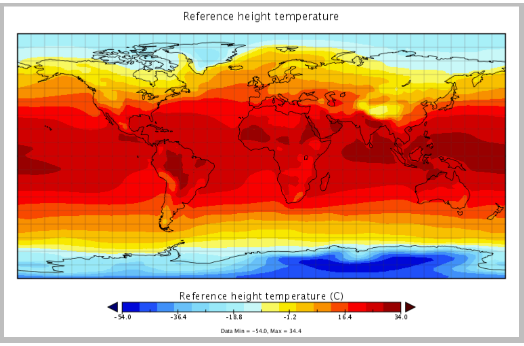

Introduction to Uncertainty Analysis

Michael S. Eldred, Richard V. Field

Sandia National Laboratories, Albuquerque, NM

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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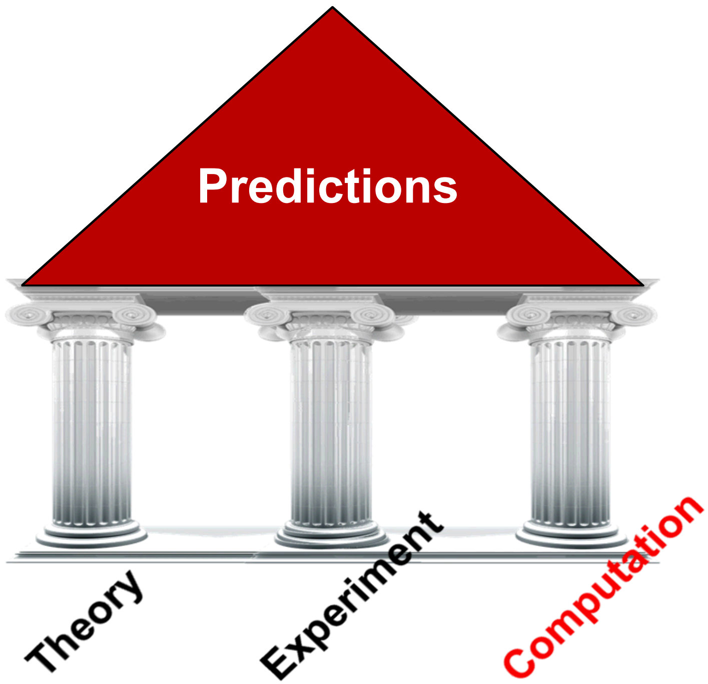
Credible Prediction in Science and Engineering

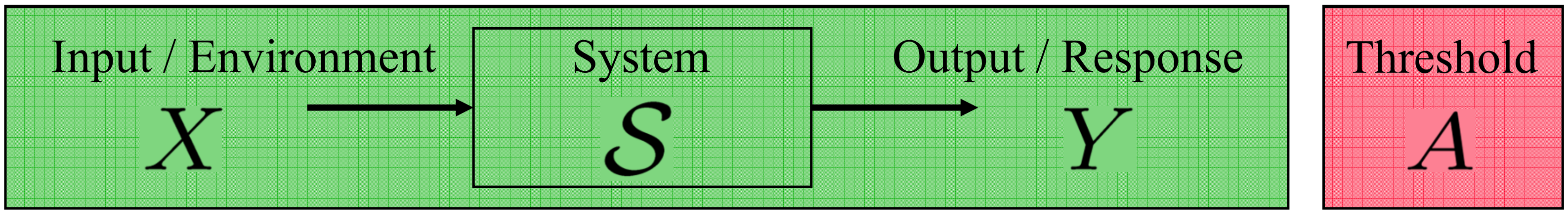


- Computational science now provides the "third pillar" of scientific discovery
- Predictive computational models, enabled by theory and experiment, can help:
  - Predict and analyze scenarios, including in untestable regimes
  - Explore operational ranges to assess risk and suitability
  - Design through virtual prototyping
  - Test theories for complex scenarios
  - Guide physical experiments
- *Answer what-if? when experiments infeasible…*

To make simulation credible for scientific, engineering, & policy decisions, we must:

- **Ask critical questions of theory, experiments, simulation**
- **Use V&V and model management processes to ensure quality and rigor**
- **Manage uncertainties and use tools for UQ, calibration, optimization**

Uncertainty in Complex Systems

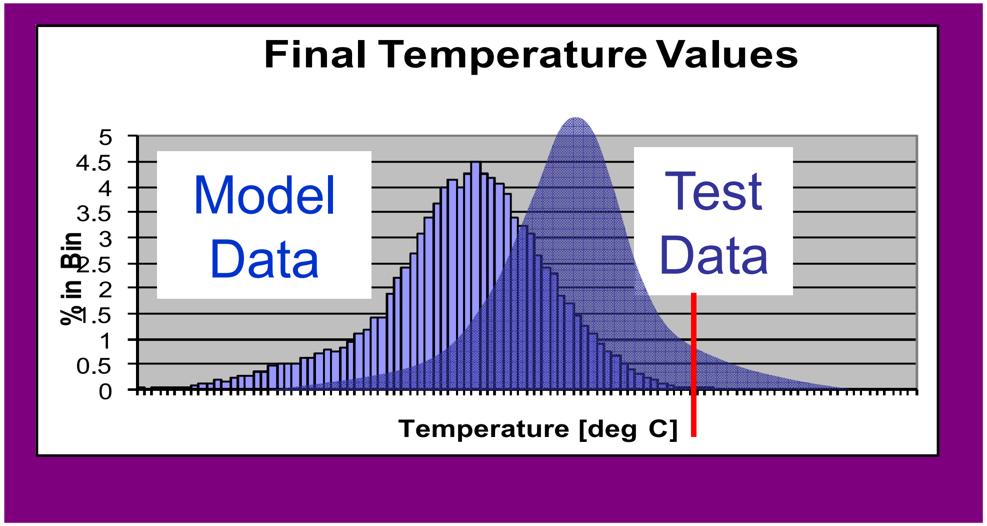


- Uncertainty in some features of ***X***, *S*, and/or ***A***
  - Sources include: inherent variability (aleatory) and ignorance (epistemic)
  - Present in: model predictions and experimental observations
- Probabilistic models are one way to quantify the effects of uncertainty on output properties
  - Based on data, theory, and/or expert opinion
  - Calibration / validation of probabilistic models is possible (and necessary)
- Probabilistic representation for input and/or system description implies probabilistic representation for output
  → predictions of system performance with quantified uncertainties

Uncertainties in Simulation and Validation

A *few* uncertainties affecting computational model output/results:

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

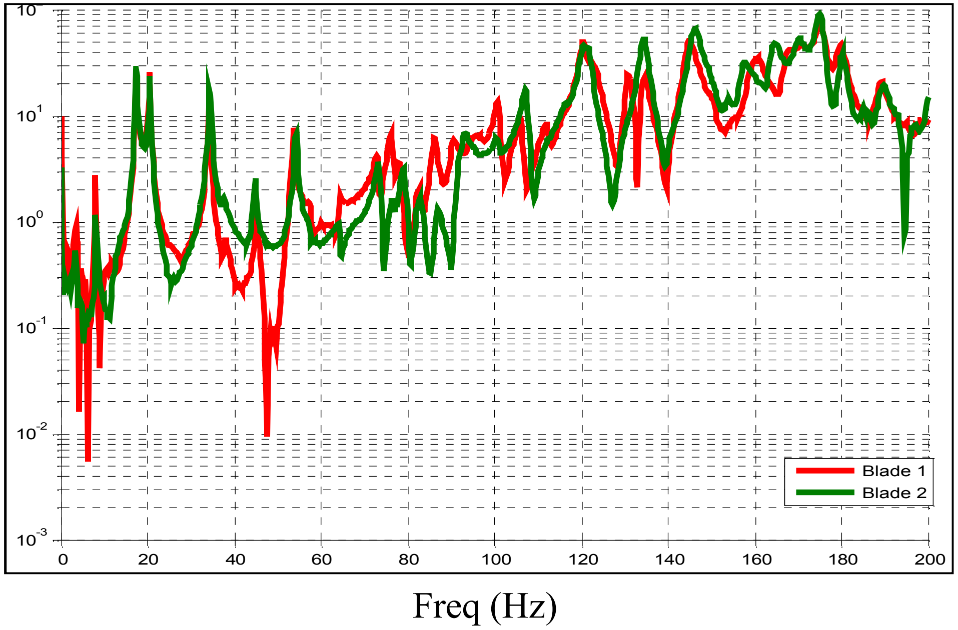


The effect of these on model outputs should be integral to an analyst's deliverable: *best estimate PLUS uncertainty!*

Example of Unit-to-Unit Variability

Wind turbine blade

Response FRFs of two "identical" blades



Probability Basics

Random Variables: Definitions

- Let X be a random variable
  - Cumulative distribution function (CDF)

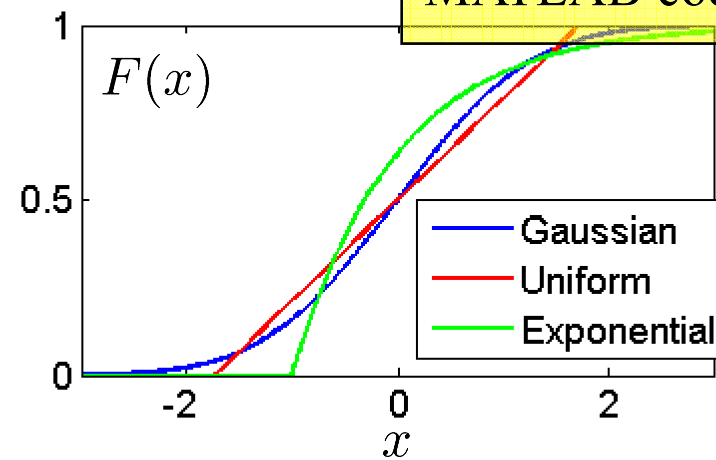
$$F(x) = \Pr(X \leq x), \ -\infty < x < \infty$$

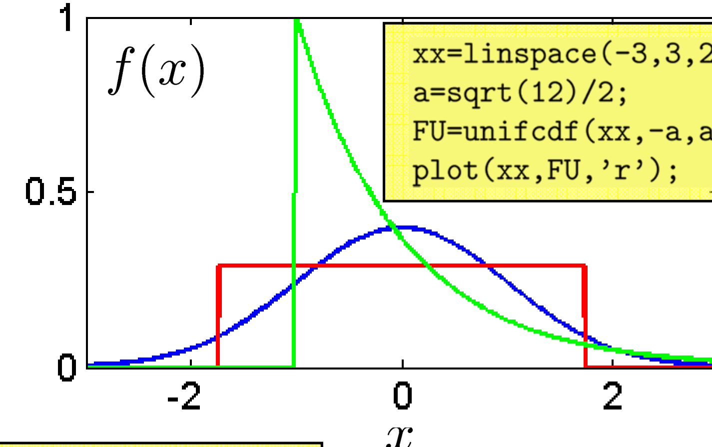
  - Probability density function (PDF)

$$f(x) = \frac{\mathrm{d}}{\mathrm{d}x} F(x)$$

- The 3 CDFs/PDFs of X shown here have zero mean and unit variance

MATLAB code






```
xx=linspace(-3,3,200);
a=sqrt(12)/2;
FU=unifcdf(xx,-a,a);
plot(xx,FU,'r');
```

```
fU=unifpdf(xx,-a,a);
plot(xx,fU,'r');
```

Some Properties of Random Variables: Statistical Moments

- Absolute moments of X

$$E[X^p] = \int_{-\infty}^{\infty} x^p \, f(x) \, dx, \;\; p \geq 1$$

$p = 1$ gives the mean of X, denoted by μ

- Central moments of X

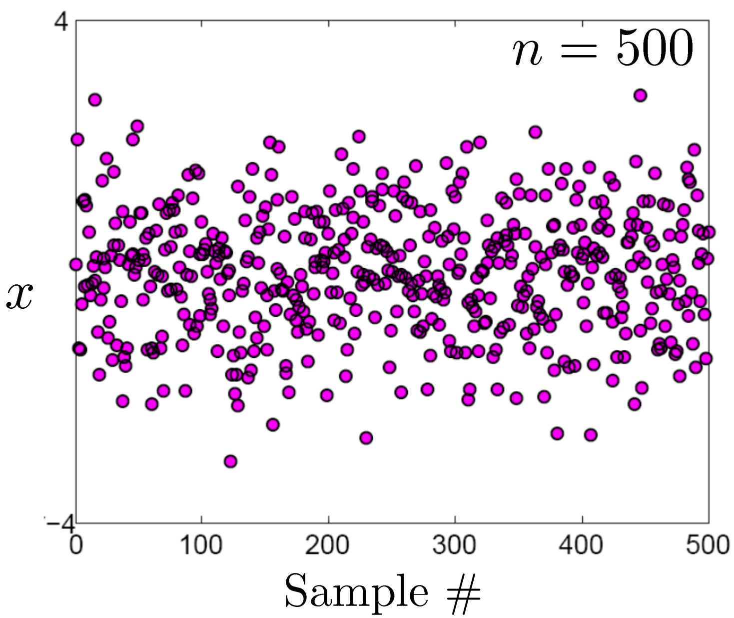
$$E[(X - \mu)^p] = \int_{-\infty}^{\infty} (x - \mu)^p \, f(x) \, dx$$

$p = 2$ gives the variance of X, denoted by σ^2

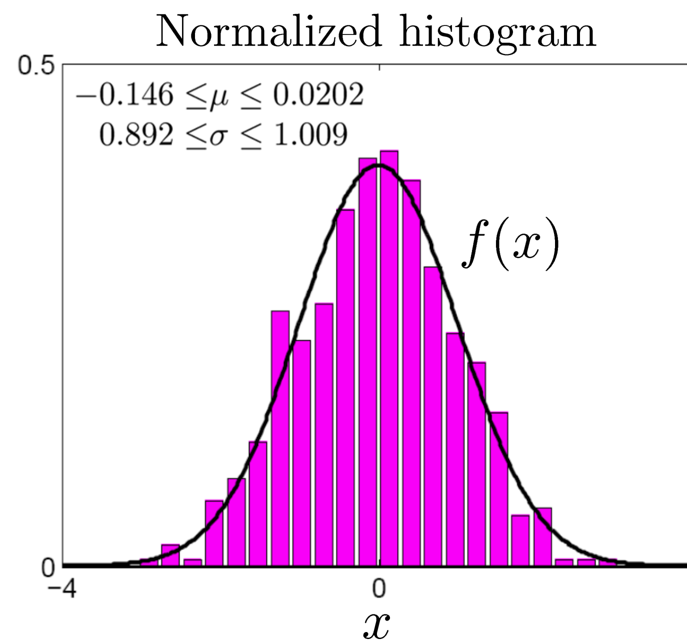
- Comments
  - For applications, we often only know some of the moments (statistics) of X
  - X is only partially defined by its moments (a complete definition requires the PDF or CDF)

Random Variables: Sample Generation

n independent samples of Gaussian random variable *X* with $\mu = 0$ and $\sigma = 1$ by Monte Carlo simulation




```
x=randn(500,1);
plot([1:500],x);
```




```
hist(x,25);hold
xx=linspace(-4,4,250);
f=normpdf(xx,0,1);
plot(xx,f)
```

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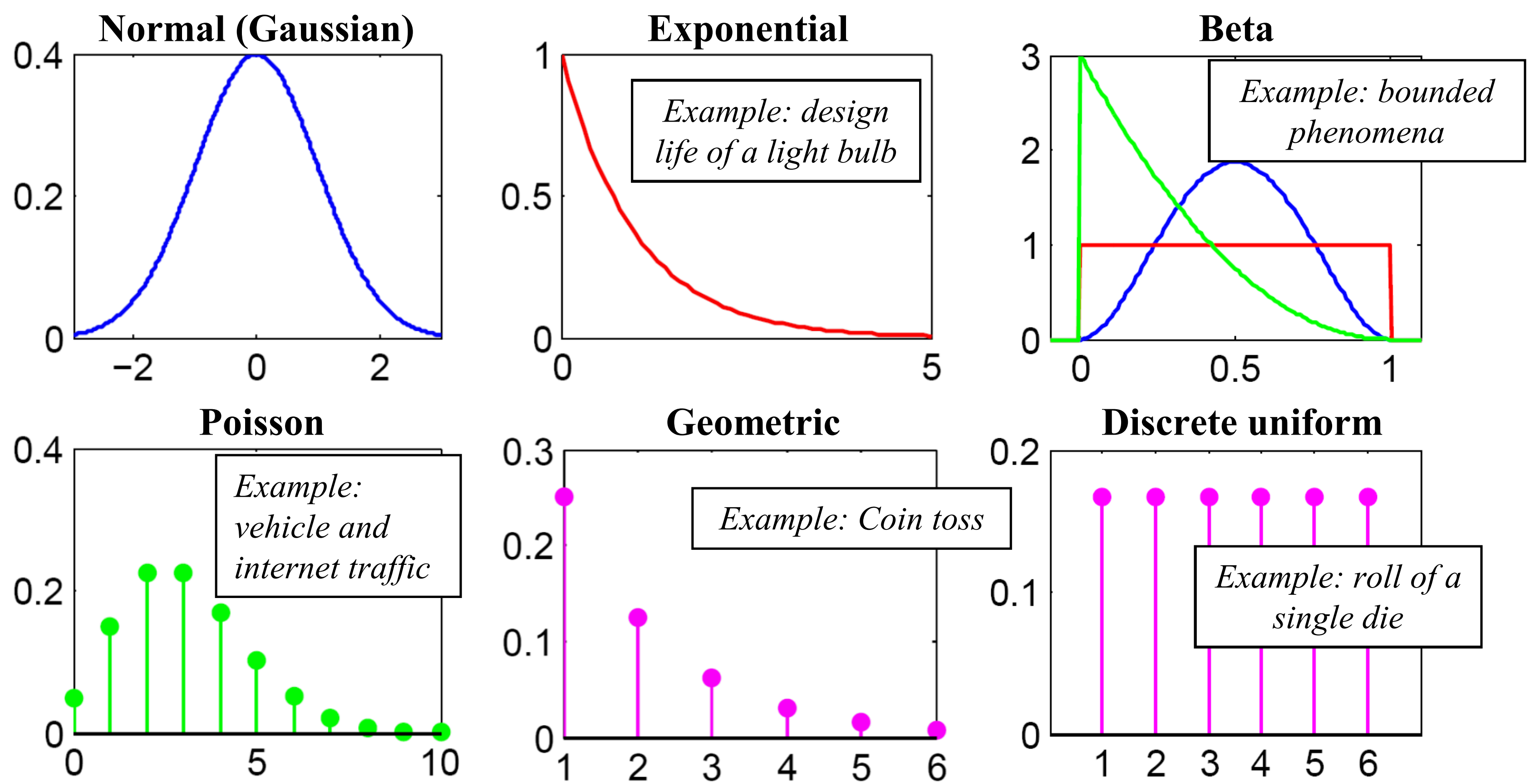
Some Commonly Used PDFs



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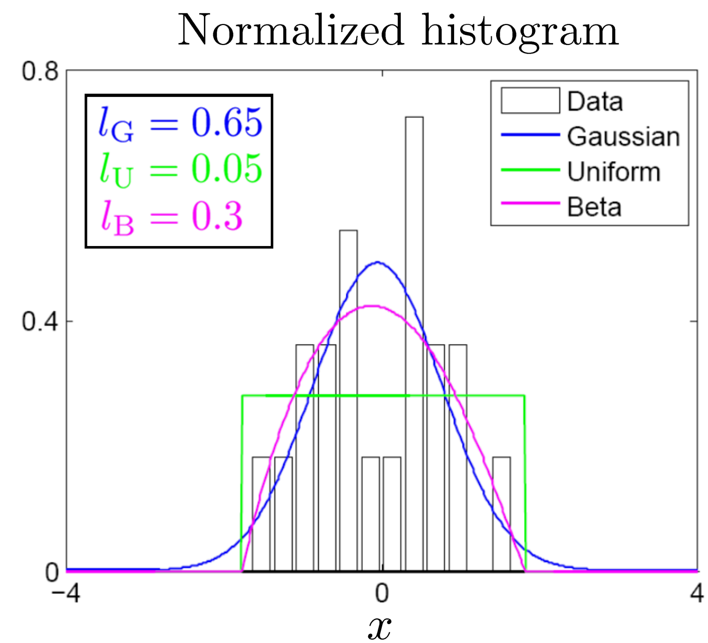
Random Variables: Modeling Techniques

- 20 independent samples of X
  - $x_1, x_2, \ldots, x_{20}$
- Statistical considerations
  - Method of moments
  - Method of maximum likelihood
- Physical considerations
  - Is X continuous or discrete?
  - Is X bounded? Semi-bounded?
  - Is PDF of X symmetric about $x = 0$?
- Other considerations
  - Conservatism / ease of use
  - What are the consequences / tradeoffs between the different models?




```
[thN1,thN2]=normfit(x);
lG=prod(normpdf(x,thN1,thN2));
```

Tools: Matlab, Minitab, Excel, JMP

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Two or More Random Variables: Random Vectors

- Let $\boldsymbol{X} = (X_1, X_2)$ be a random vector
  - Joint CDF

$$F(x_1, x_2) = \Pr(X_1 \leq x_1 \cap X_2 \leq x_2)$$

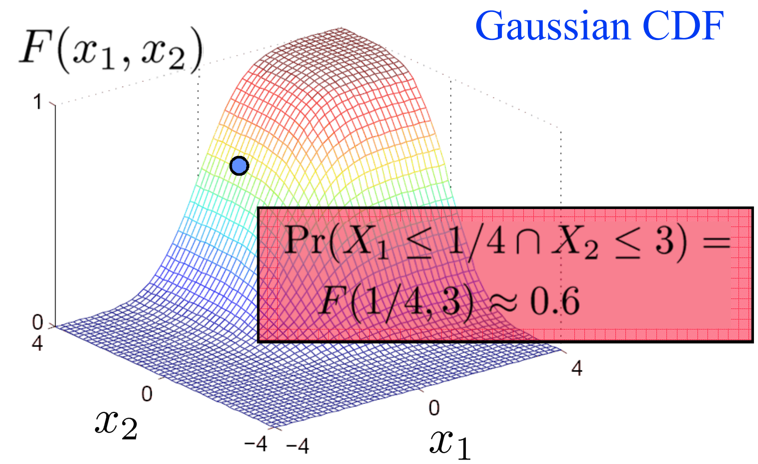
  - Joint PDF

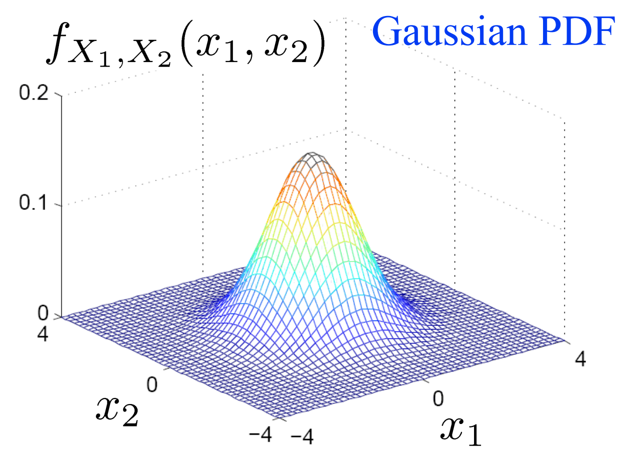
$$f_{X_1,X_2}(x_1, x_2) = \frac{\partial^2}{\partial x_1 \, \partial x_2} F(x_1, x_2)$$

  - Special case: X_1 and X_2 are independent (this is a very strong condition)

$$f_{X_1,X_2}(x_1, x_2) = f_{X_1}(x_1) \cdot f_{X_2}(x_2)$$

$$\Pr(X_1 \leq 1/4 \cap X_2 \leq 3) = \Pr(X_1 \leq 1/4) \cdot \Pr(X_2 \leq 3)$$





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Random Vectors: Correlation / Covariance

- Correlation of $\boldsymbol{X} = (X_1, X_2)$

$$\mathrm{Corr}(X_1, X_2) = \mathrm{E}[X_1\, X_2]$$

- Covariance of $\boldsymbol{X} = (X_1, X_2)$

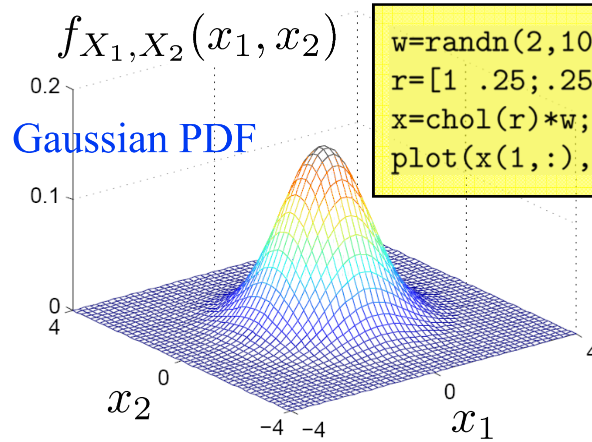
$$\mathrm{Cov}(X_1, X_2) = \mathrm{E}[(X_1 - \mu_1)\,(X_2 - \mu_2)]$$

$$\rho = \frac{\mathrm{Cov}(X_1, X_2)}{\sqrt{\mathrm{Cov}(X_1, X_1) \cdot \mathrm{Cov}(X_2, X_2)}}$$

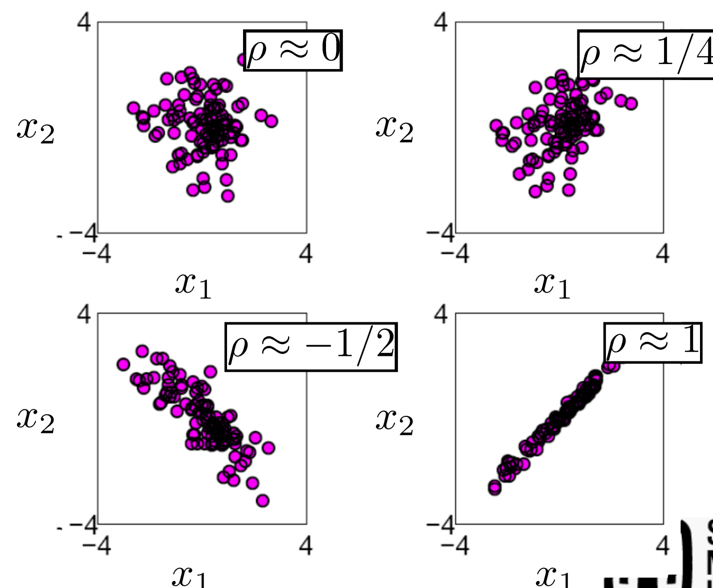
- Special case: X_1 and X_2 are uncorrelated

$$\mathrm{Cov}(X_1, X_2) = 0$$

This does not mean X_1 and X_2 are independent!




```
w=randn(2,100);
r=[1 .25;.25 1];
x=chol(r)*w;
plot(x(1,:),x(2,:),'o')
```

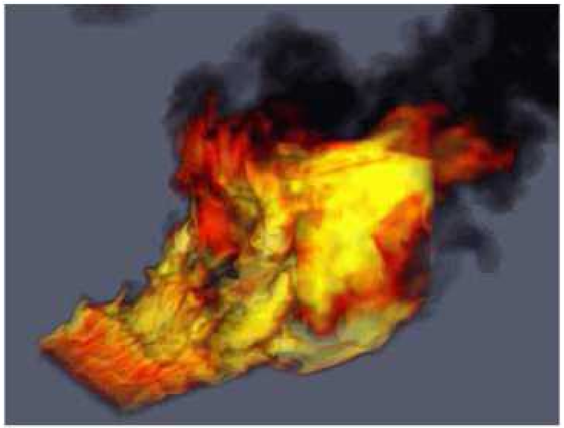


UQ Methods

Current DOE Mission Areas: UQ R&D and Deployment

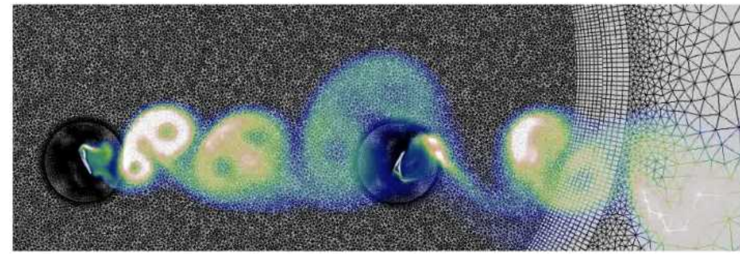
Stockpile Stewardship (NNSA ASC)

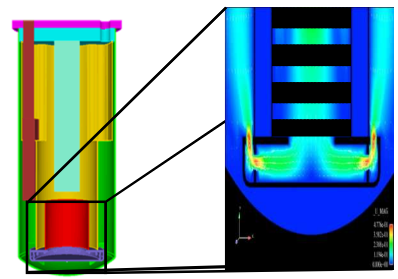
Safety in abnormal environments

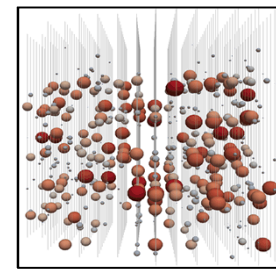


Energy (ASCR, EERE, NE CASL)

Wind turbines, nuclear reactors







Climate (SciDAC, CSSEF)

Ice sheet modeling, CISM, CESM, ISSM

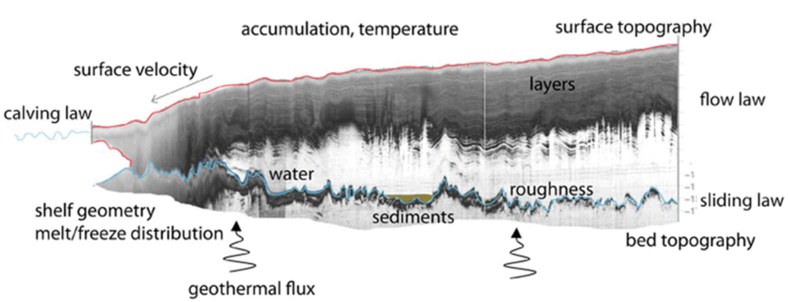
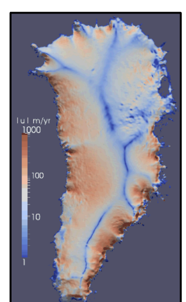
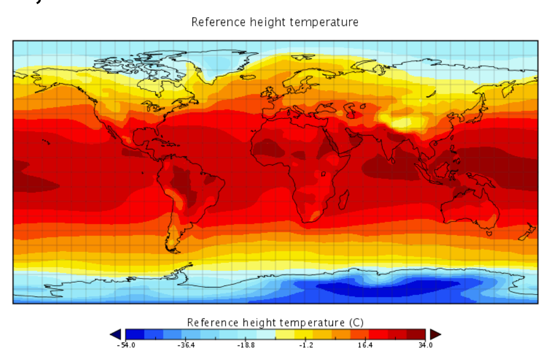


Figure 1: Schematic of observations, boundary conditions, and processes affecting ice sheet initialization.

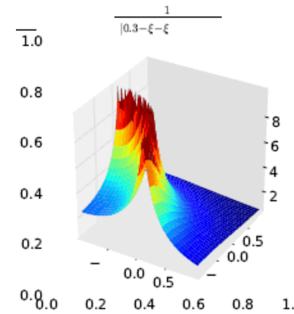




Emphasis on Scalable Methods for High-fidelity UQ on HPC

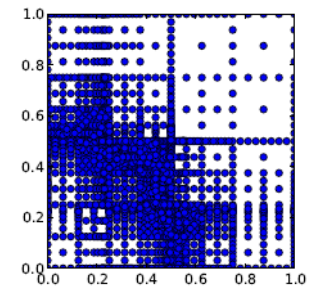
Key Challenges:

- Severe simulation budget constraints (e.g., a handful of HF runs)
- Moderate to high-dimensional in random variables: $O(10^1)$ to $O(10^2)$ [post KLE]
- Compounding effects:
  - Mixed aleatory-epistemic uncertainties (→ nested iteration)
  - Requirement to evaluate probability of rare events (e.g., safety criteria)
  - Nonsmooth responses (→ difficulty with fast converging spectral methods)



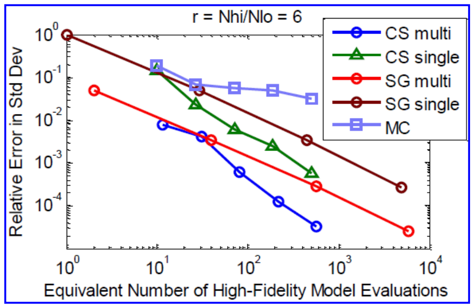
Core UQ Capabilities:

- Sampling methods: LHS, MC, QMC, incremental
- Reliability methods: local (MV, AMV+, FORM, …), global (EGRA, GPAIS, POFDarts)
- Stochastic expansion methods: polynomial chaos, stochastic collocation
- Epistemic methods: interval estimation, Dempster-Shafer evidence



Research Thrusts:

- Compute dominant uncertainty effects despite key challenges above
- Scalable UQ foundation
  - Adaptive refinement, Adjoint enhancement, Sparsity detection
- Leverage his foundation within component-based meta-iteration
  - Mixed UQ incl. model form, Multifidelity UQ, Bayesian methods



Uncertainty Quantification Algorithms in DAKOTA: New methods bridge robustness/efficiency gap

	Traditional (at Sandia)	Production	Recently released	Under dev Planned	Collabs.
Sampling	**Latin Hypercube, Monte Carlo**	**Incremental**	**Adaptive Importance**	**Bootstrap, Jackknife**	**FSU**
Reliability	***Local:* Mean Value, 1st- & 2nd-order reliability (AMV+, FORM, SORM)**	**Global reliability methods (EGRA)**	**GPAIS, POFDarts, GPs with gradient-enhancement**	**Recursive emulation, TGP**	***Local:* Notre Dame, *Global:* Vanderbilt**
Stochastic expansion		**Polynomial chaos, stoch collocation (regression,**	**Dimension-adaptive p-/h-refinement, grad-enhancement, sparsity detection**	**Local adapt refinement, adjoint EE, discrete vars**	**Stanford, Utah**
Epistemic & Mixed UQ	**Interval-valued/ 2nd-order prob. w/nested sampling**		**Opt-based interval est, Dempster-Shafer, discrete model forms**	**Discrete GPs, Imprec. probability**	**Arizona St**
Bayesian			**Emulator based MCMC with QUESO, GPMSA**	**model selection, multifidelity**	**LANL, UT Austin**
Other			**Efficient subspace method, Morris-Smale topology**	**Rand fields / stoch proc, Moment meth**	**NCSU, Utah, Cornell, Maryland**

Research: Scalability, Robustness, Goal-orientation

Adv. Deployment

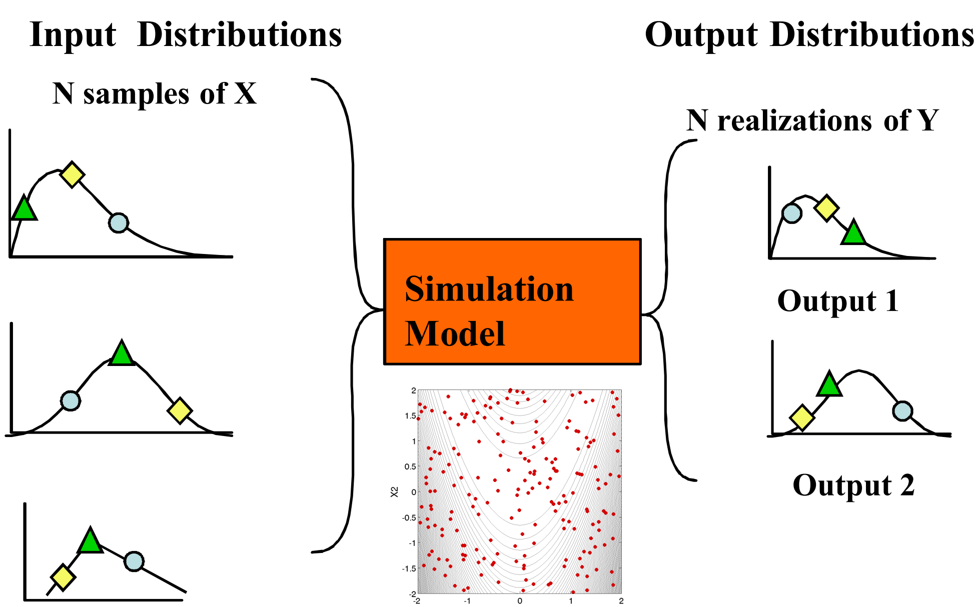
Fills Gaps

Sampling

Starting from distributions on the uncertain input values, draw observations from each distribution, pair samples, and execute the model for each pairing
→ *ensemble of results yields distributions of the outputs*

- Monte Carlo: basic random sampling
- Pseudo Monte Carlo: Latin Hypercube Sampling (LHS)
- Quasi Monte Carlo: Halton, Hammersley, Sobol sequences
- Orthogonal arrays, Centroidal Voronoi Tesselation (CVT), Importance Sampling

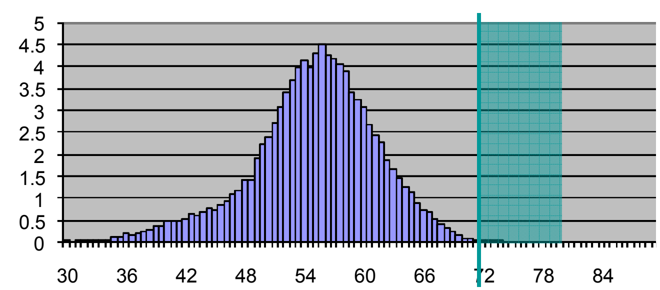
Sampling is not the most efficient UQ method, but is easy to implement, robust, & transparent.



- **sample mean and variance**

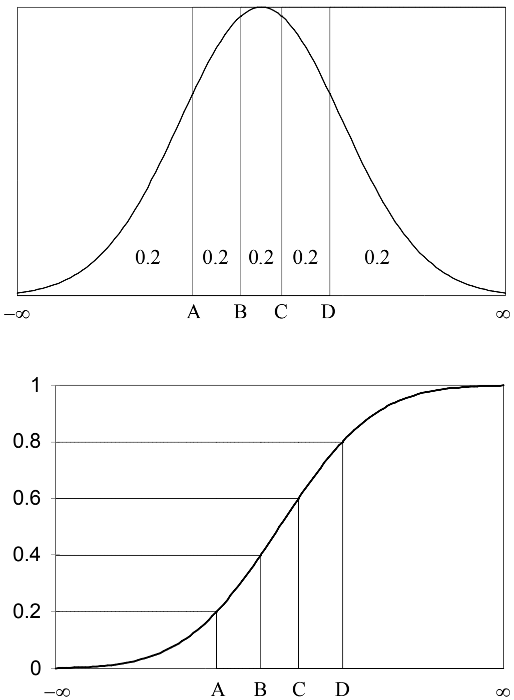
$$\bar{T} = \frac{1}{N}\sum_{i=1}^{N} T(u^i) \qquad T_{\sigma^2} = \frac{1}{N}\sum_{i=1}^{N}\left[T(u^i) - \bar{T}\right]^2$$

- **full PDF and CDF**



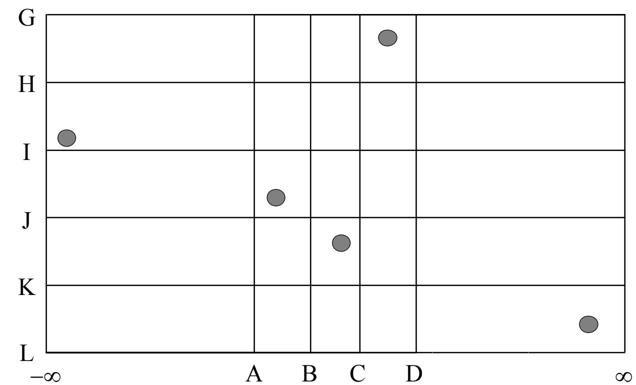
Latin Hypercube Sampling

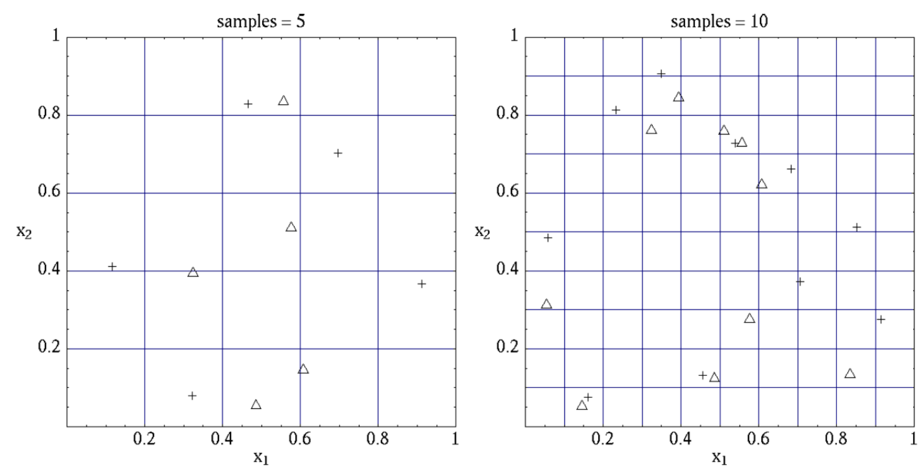
- LHS is stratified random sampling among equal probability bins for all 1-D projections of an n-dimensional set of samples.
  - Early work by McKay and Conover
  - Restricted pairing by Iman → enforce prescribed input correlations



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

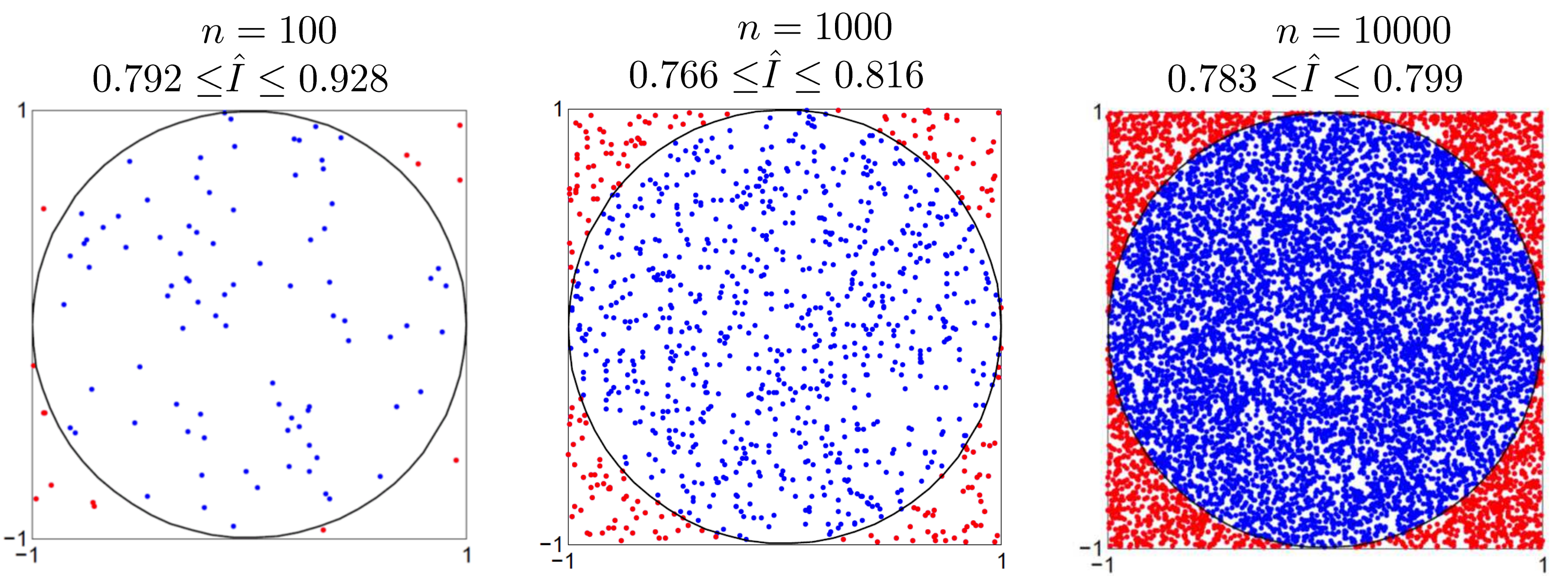
A possible LHS for n=2, N=5 with X1 = normal and X2 = uniform





Simple Monte Carlo Example

- Ratio of area of an inscribed circle to the area of a square



$$
\begin{aligned}
I &= \frac{1}{r^2} \int_0^r \sqrt{r^2 - x^2}\, \mathrm{d}x \\
&= \frac{\pi}{4} \approx 0.785
\end{aligned}
$$

UQ Methods: Reliability

UQ with Reliability Methods: Mean Value Method

Linear approximation for first two moments:

$$\begin{aligned} \mu_g &= g(\mu_{\mathbf{x}}) \\ \sigma_g^2 &= \sum_i \sum_j Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}}) \end{aligned}$$

Projection of moments for reliability indices:

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

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

Normality assumption:

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

Rough statistics

UQ with Reliability Methods: Most Probable Point (MPP) Search Methods

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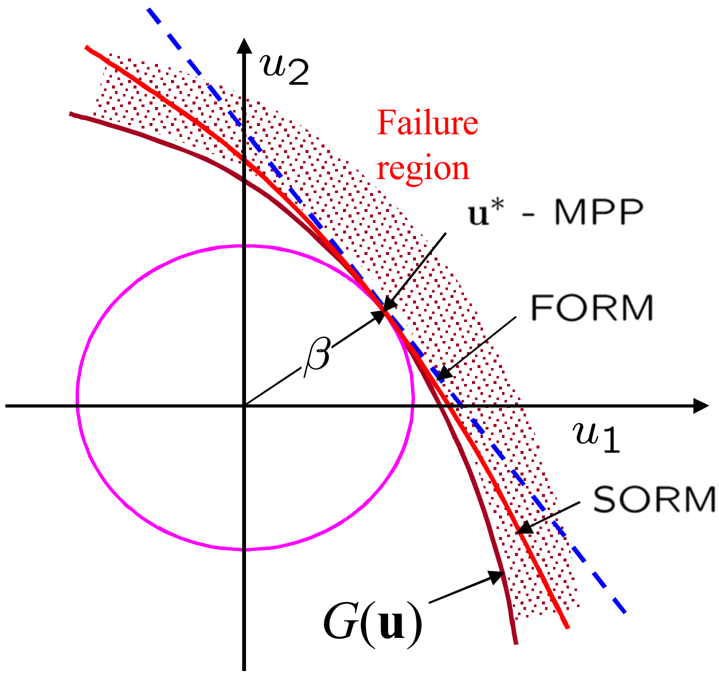
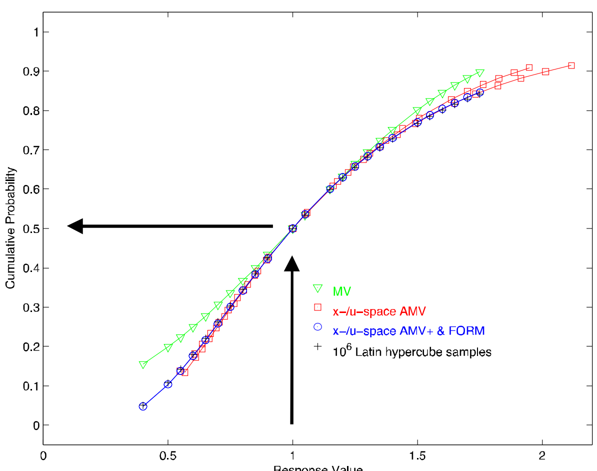


Reliability Index Approach (RIA)

$$\begin{array}{ll} \text{minimize} & \mathbf{u}^T\mathbf{u} \\ \text{subject to} & G(\mathbf{u}) = \bar{z} \end{array}$$

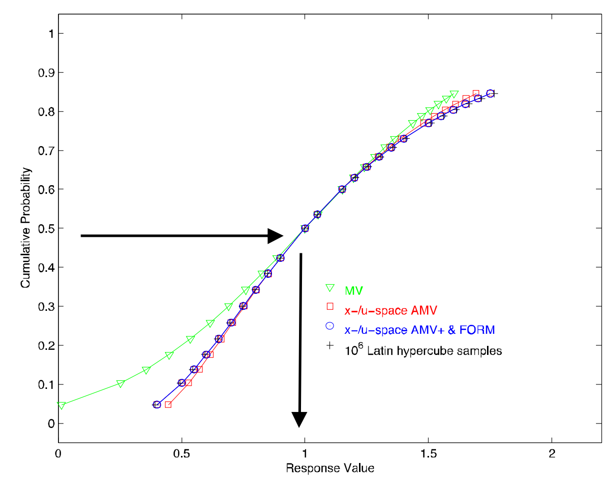
Find min dist to *G* level curve
Used for fwd map *z* → *p/β*



Performance Measure Approach (PMA)

$$\begin{array}{ll} \text{minimize} & \pm G(\mathbf{u}) \\ \text{subject to} & \mathbf{u}^T\mathbf{u} = \bar{\beta}^2 \end{array}$$

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

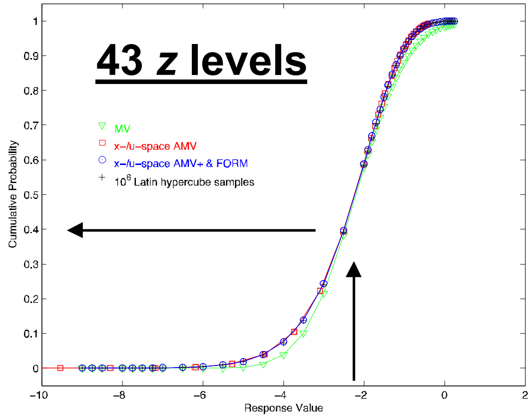


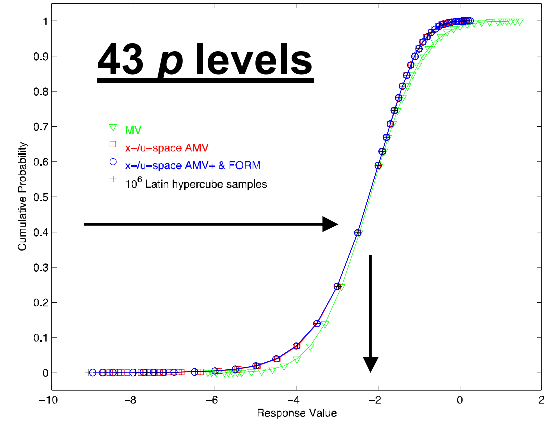
Nataf x → u:

$$\Phi(z_i) = F(x_i)$$
$$\mathbf{z} = \mathbf{L}\mathbf{u}$$

Reliability Algorithm Variations:

Sample Algorithm Performance: short column test





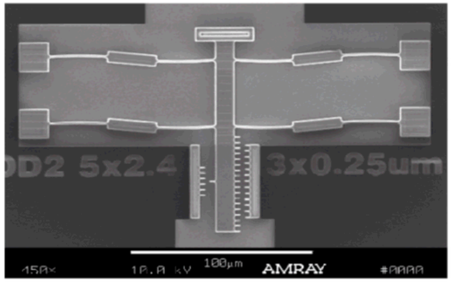
RIA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF p Error Norm	Target z Offset Norm
MVFOSM	1	1	0.1548	0.0
MVSOSM	1	1	0.1127	0.0
x-space AMV	45	45	0.009275	18.28
u-space AMV	45	45	0.006408	18.81
x-space AMV^2	45	45	0.002063	2.482
u-space AMV^2	45	45	0.001410	2.031
x-space AMV+	192	192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

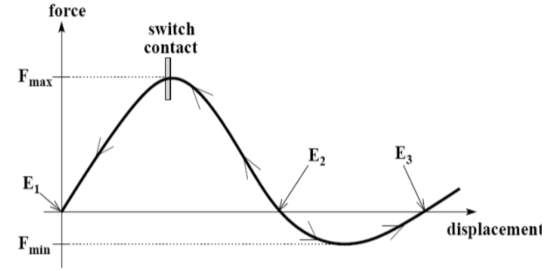
PMA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF z Error Norm	Target p Offset Norm
MVFOSM	1	1	7.454	0.0
MVSOSM	1	1	6.823	0.0
x-space AMV	45	45	0.9420	0.0
u-space AMV	45	45	0.5828	0.0
x-space AMV^2	45	45	2.730	0.0
u-space AMV^2	45	45	2.828	0.0
x-space AMV+	171	179	0.0	0.0
u-space AMV+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

Note: 2nd-order PMA with prescribed p level requires $\beta(p)$ inversion

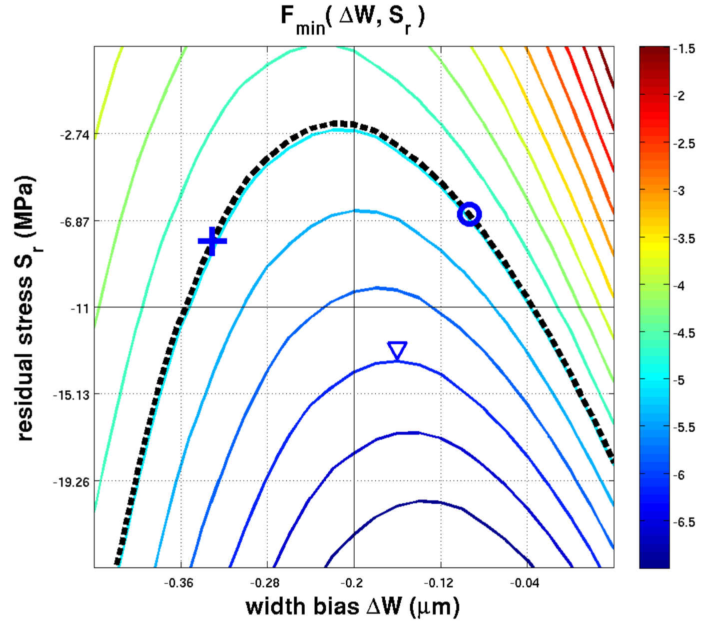
Solution-Verified Reliability Analysis and Design of MEMS

- Problem: MEMS subject to substantial variabilities
  - Material properties, manufactured geometry, residual stresses
  - Part yields can be low or have poor durability
  - Data can be obtained → aleatory UQ → probabilistic methods
- Goal: account for both uncertainties and errors in design
  - Integrate UQ/OUU (DAKOTA), ZZ/QOI error estimation (Encore), adaptivity (SIERRA), nonlin mech (Aria) → MESA application
  - Perform soln verification in automated, parameter-adaptive way
  - Generate fully converged UQ/OUU results at lower cost





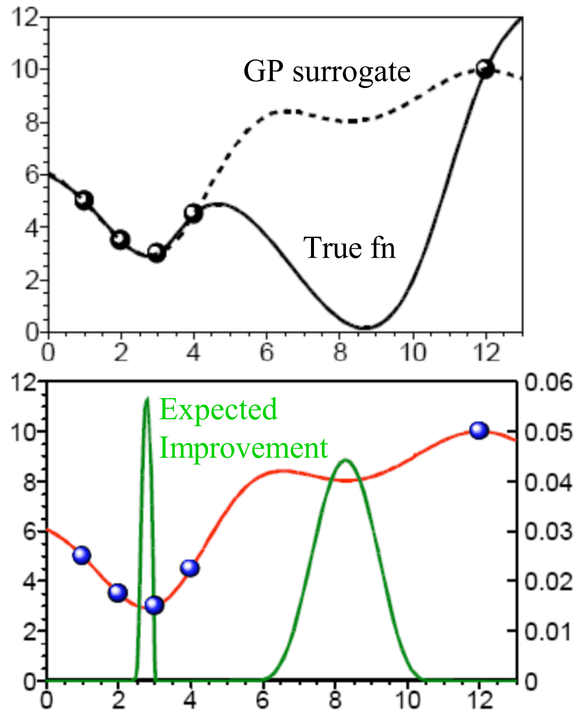
- **AMV^2+ and FORM converge to different MPPs (+ and o, respectively)**
- **Issue: high nonlinearity leading to multiple legitimate MPP solns.**
- **Challenge: design optimization may tend to seek out regions encircled by the failure domain. 1st-order and even 2nd-order probability integrations can experience difficulty with this degree of nonlinearity. Optimizers can/will exploit this model weakness.**



Parameter study over 3σ uncertain variable range for fixed design variables d_M*. ***Dashed black line denotes $g(x) = F_{min}(x) = -5.0$.***

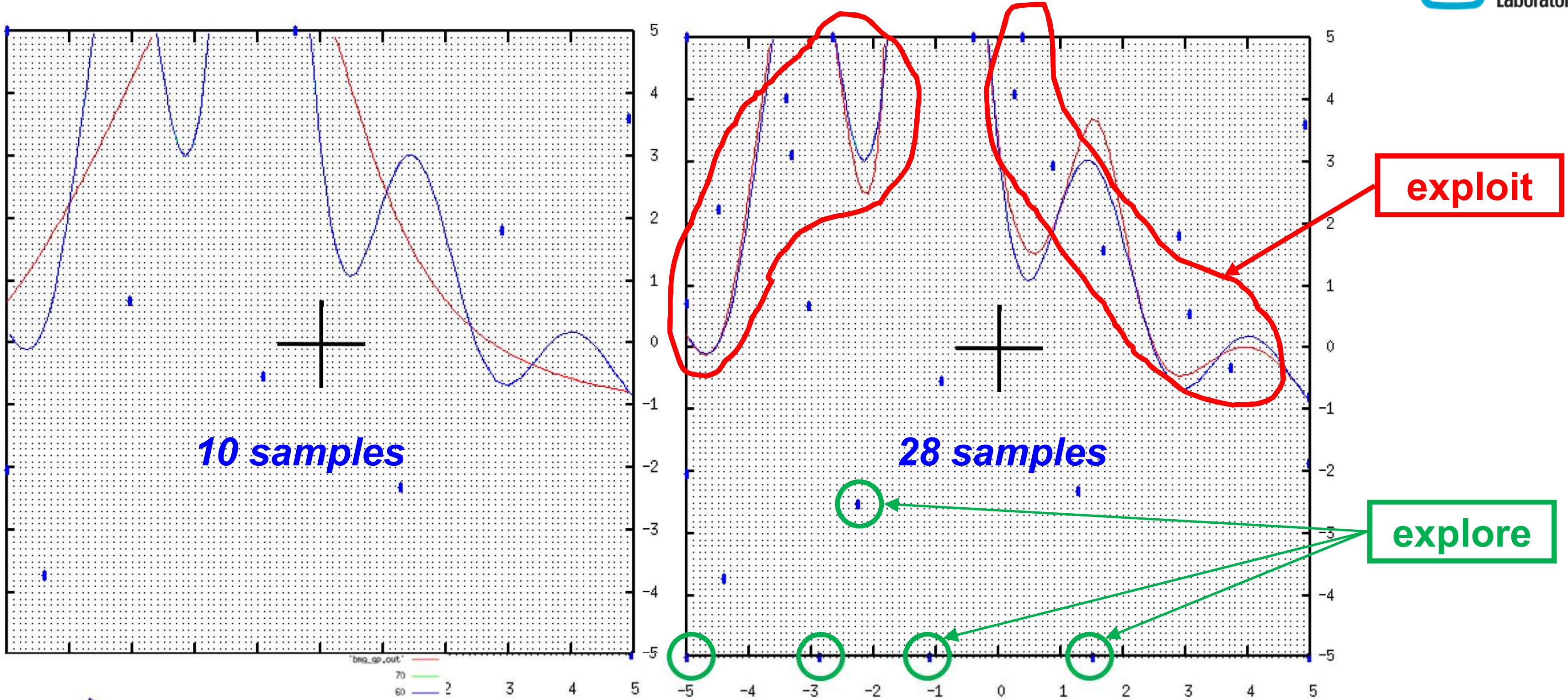
Efficient Global Reliability Analysis (EGRA)

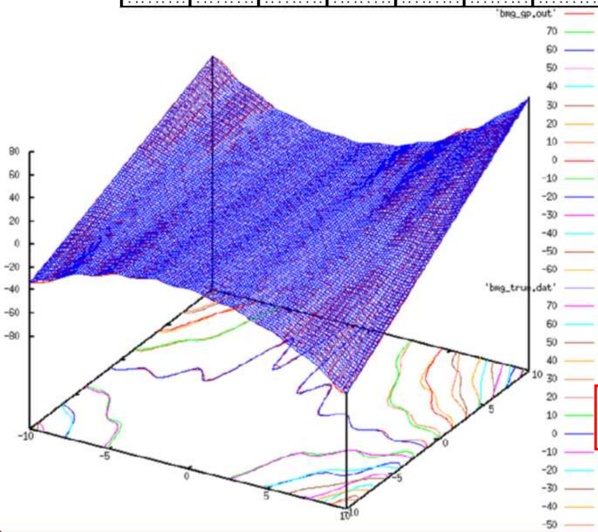
- **Address known failure modes of local reliability methods:**
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. fail to accurately estimate probability at MPP
- **Based on EGO (surrogate-based global opt.),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



From Jones, Schonlau, Welch, 1998

Efficient Global Reliability Analysis





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

UQ Methods: Stochastic Expansions

Non-Intrusive Stochastic Expansions:

Polynomial Chaos and Stochastic Collocation

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Polynomial chaos: spectral projection using orthogonal polynomial basis fns

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

using

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

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

- Estimate α_j using regression or numerical integration: sampling, tensor quadrature, sparse grids, or cubature

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

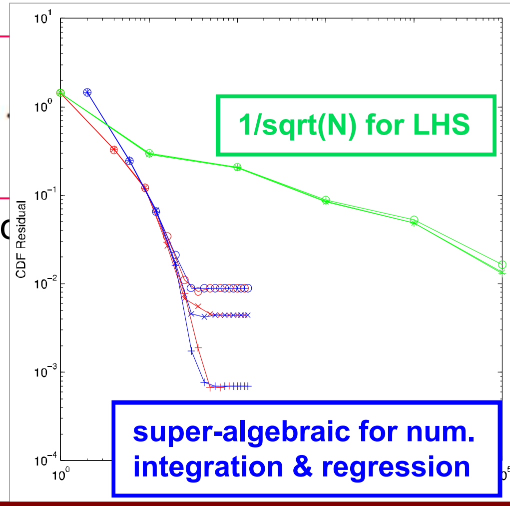
Stochastic collocation: instead of estimating coefficients for known basis functions, form interpolants for known coefficients

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

- ***Global:*** Lagrange (values) or Hermite (values+derivatives)
- ***Local:*** linear (values) or cubic (values+gradients) splines

$$L_j = \prod_{\substack{k=1 \\ k \neq j}}^{m} \frac{\xi - \xi_k}{\xi_j - \xi_k} \quad \Rightarrow \quad R(\boldsymbol{\xi}) \cong \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots\right.$$

Sparse interpolants formed using Σ of tensor interp



- Tailor expansion form:
  - p-refinement: anisotropic tensor/sparse, generalized sparse
  - h-refinement: local bases with dimension & local refinement
- Method selection: fault tolerance, decay, sparsity, error est.

Approaches for forming PCE/SC Expansions

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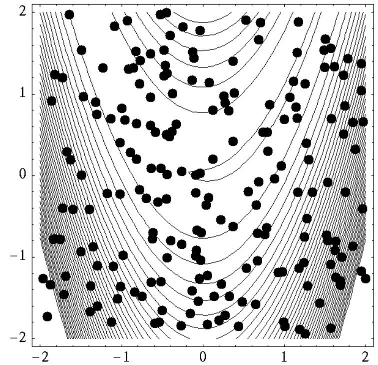
Random sampling: PCE

Expectation (sampling):

- Sample w/i distribution of ξ
- Compute expected value of product of R and each Ψ_j

Least squares regression:

- Sample w/i distribution of ξ
- Solves least squares data fit for all coefficients at once:



$$\Psi\alpha = R$$

Compressive sensing

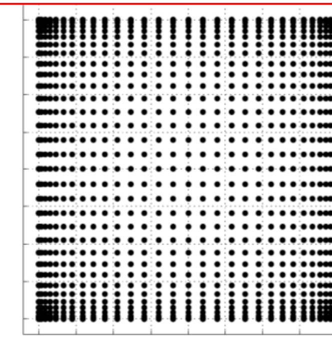
- Underdetermined systems: sparse basis pursuit for with L1 regularization

Tensor-product quadrature: PCE/SC

$$\mathscr{U}^i(f)(\xi) = \sum_{j=1}^{m_i} f(\xi_j^i)\, w_j^i$$

$$Q_{\mathbf{i}}^n f(\xi) = (\mathscr{U}^{i_1}\otimes\cdots\otimes\mathscr{U}^{i_n})(f)(\xi) = \sum_{j_1=1}^{m_{i_1}}\cdots\sum_{j_n=1}^{m_{i_n}} f\left(\xi_{j_1}^{i_1},\dots,\xi_{j_n}^{i_n}\right)\left(w_{j_1}^{i_1}\otimes\cdots\otimes w_{j_n}^{i_n}\right)$$

- **Every combination of 1-D rules**
- **Scales as *m^n***
- **1-D Gaussian rule of order *m* → integrands to order *2m – 1***
- **Assuming $R\Psi_j$ of order 2*p*, select *m = p + 1***

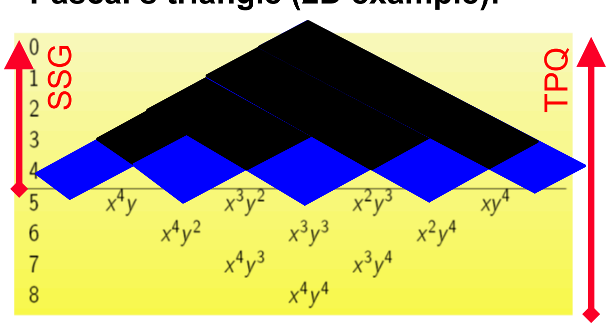


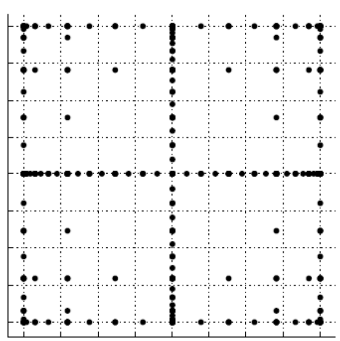
Sparse Grid: PCE/SC

$$\mathscr{A}(\mathrm{w},n) = \sum_{|\mathbf{i}|\le \mathrm{w}+n} \left(\Delta^{i_1}\otimes\cdots\otimes\Delta^{i_n}\right)$$

$$\mathscr{A}(\mathrm{w},n) = \sum_{\mathrm{w}+1\le|\mathbf{i}|\le\mathrm{w}+n} (-1)^{\mathrm{w}+n-|\mathbf{i}|}\binom{n-1}{\mathrm{w}+n-|\mathbf{i}|}\cdot\left(\mathscr{U}^{i_1}\otimes\cdots\otimes\mathscr{U}^{i_n}\right)$$

Pascal's triangle (2D example):



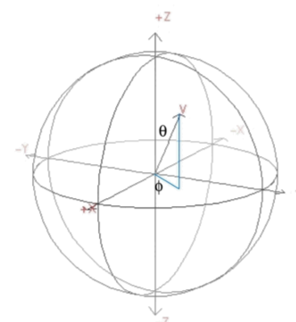


Cubature: PCE

Stroud and extensions (Xiu, Cools)

→ Low order PCE

→ global SA, anisotropy detection



Gaussian *i* = 2 → *p* = 1

$$x_{k,2r-1} = \sqrt{2}\cos\frac{2rk\pi}{n+1}, \qquad x_{k,2r} = \sqrt{2}\sin\frac{2rk\pi}{n+1}$$

Arbitrary PDF $t^{(k)} = \frac{1}{\gamma}\left[\sqrt{\gamma c_1}x^{(k)} - \delta\right]$

Adaptive Collocation Methods: Generalized Sparse Grids

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Polynomial order (p-) refinement approaches:

- **Uniform:** *isotropic* tensor/sparse grids
  - *Increment grid:* increase order/level, ensure change (restricted growth in nested rules)
  - *Assess convergence:* L^2 change in response covariance
- **Dimension-adaptive:** *anisotropic* tensor/sparse grids

$$\mathrm{w}\underline{\gamma} < \mathbf{i} \cdot \gamma \leq \mathrm{w}\underline{\gamma} + |\gamma|$$

  - **PCE/SC:** variance-based decomp. → total Sobol' indices → anisotropy
  - **PCE:** spectral coefficient decay rates → anisotropy
- **Goal-oriented dimension-adaptive:** *generalized* sparse grids
  - **PCE/SC:** change in QOI induced by trial index sets on active front

1. ***Initialization:*** Starting from reference grid (often w = 0 grid), define active index sets using admissible forward neighbors of all old index sets.

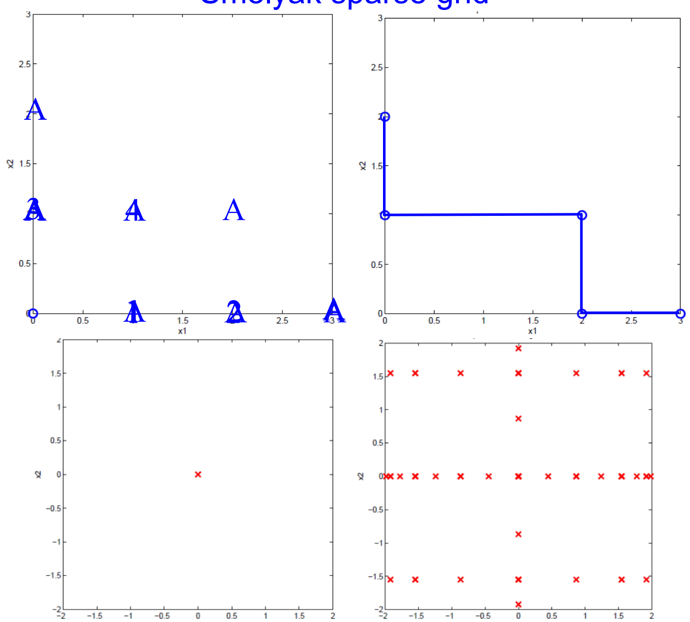
2. ***Trial set evaluation:*** For each trial index set, evaluate tensor grid, form tensor expansion, update combinatorial coefficients, and combine with reference expansion. Perform necessary bookkeeping to allow efficient restoration.

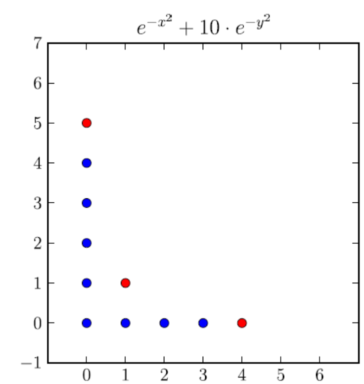
3. ***Trial set selection:*** Select trial index set that induces largest change in statistical QOI.

4. ***Update sets:*** If largest change > tolerance, then promote selected trial set from active to old and compute new admissible active sets; return to 2. If tolerance is satisfied, advance to step 5.

5. ***Finalization:*** Promote all remaining active sets to old set, update combinatorial coefficients, and perform final combination of tensor expansions to arrive at final result for statistical QOI.

Smolyak sparse grid

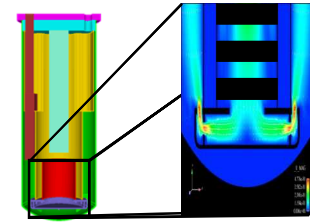




(Gerstner, 2003)

Fine-grained control: frontier not limited by prescribed shape of index set constraint

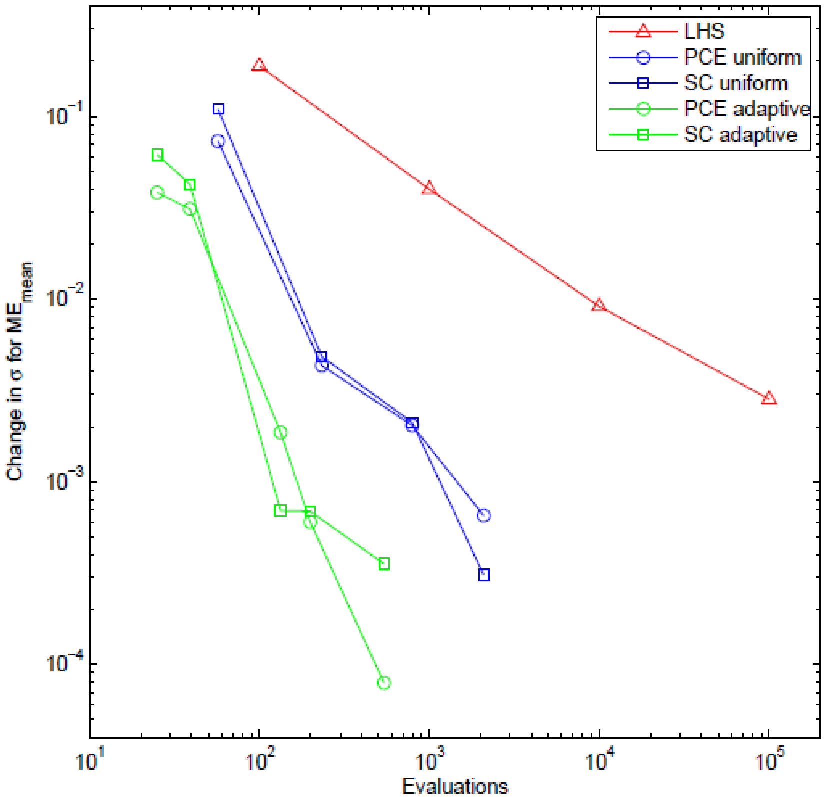
Application Deployment (CASL)



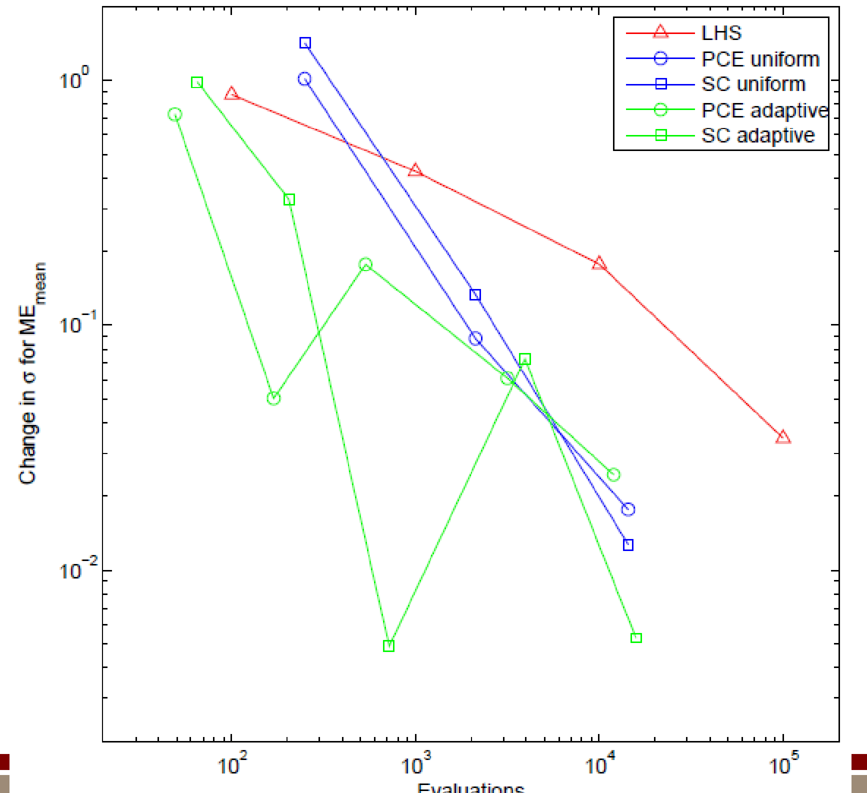
Application: Nuclear reactor cores experience localized boiling, which leads to CRUD (Chalk River Unidentified Deposit). These deposits result in undesirable power shifts (CIPS) within the core. Statistics of mass evaporation (ME) rate are of interest.

Methodology: PCE/SC with uniform/adaptive refinement compared to LHS

Plant A (n=4, smooth, mild anisotropy)



Plant B (n=10, discontinuous, high anisotropy)



ASCR: VAWT with Uncertain Gust Loading

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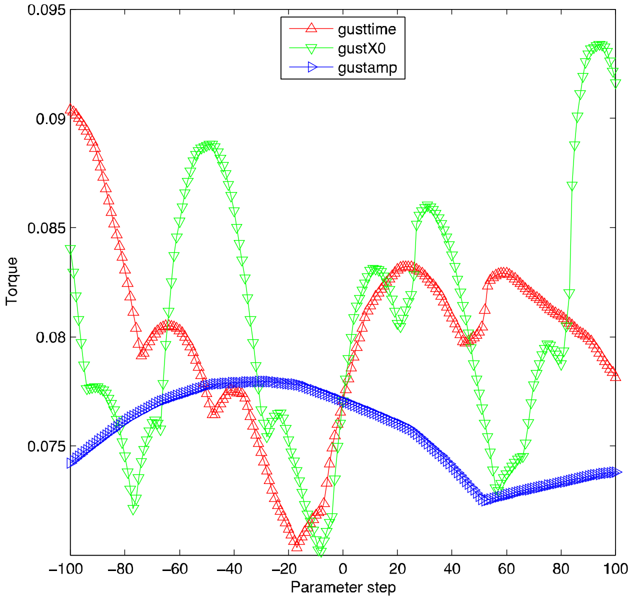
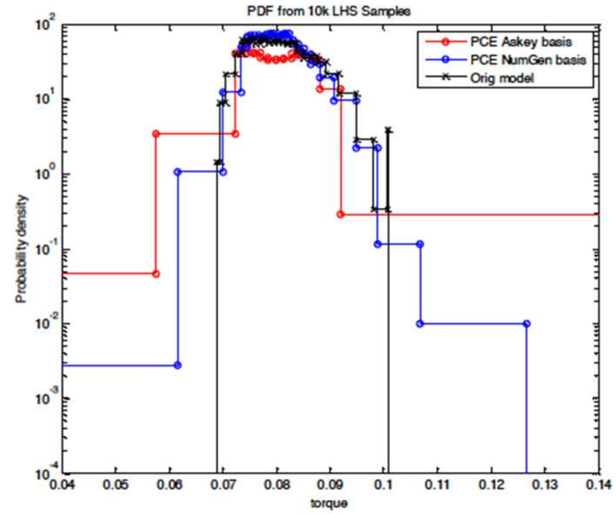
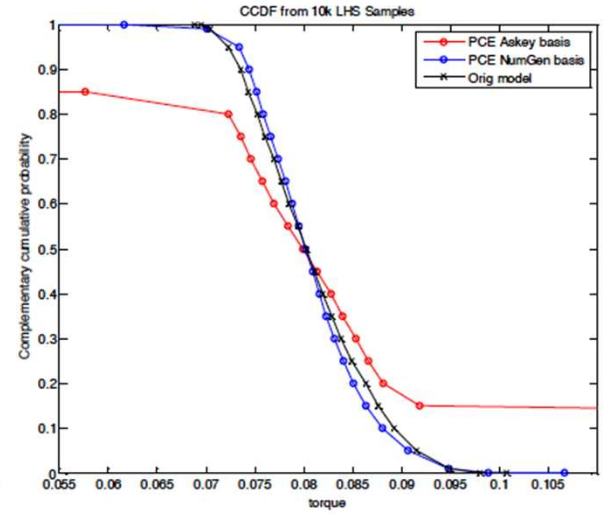
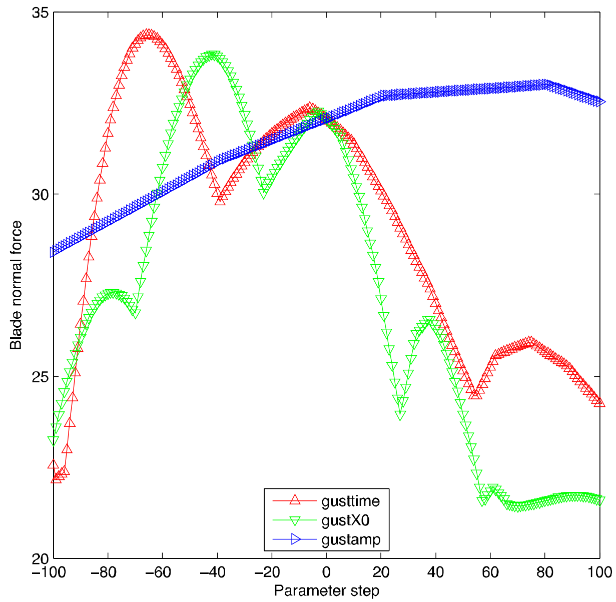
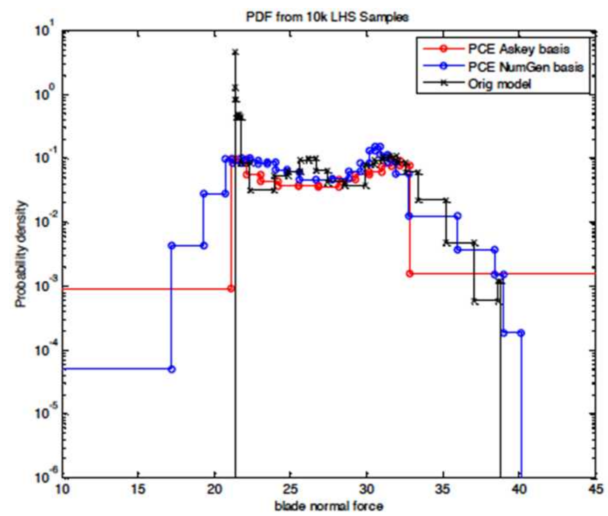
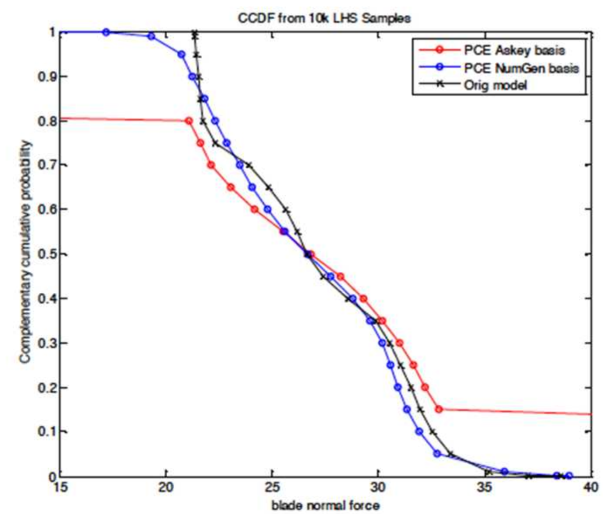








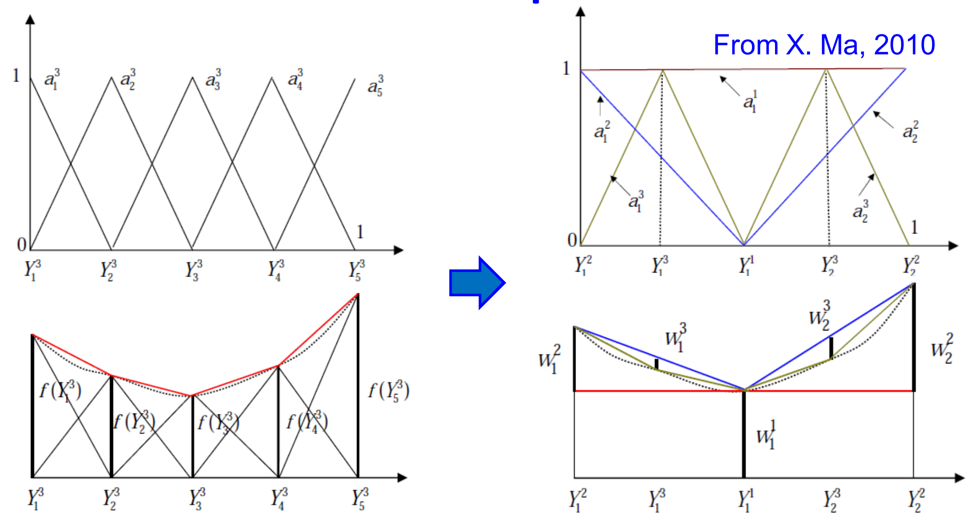




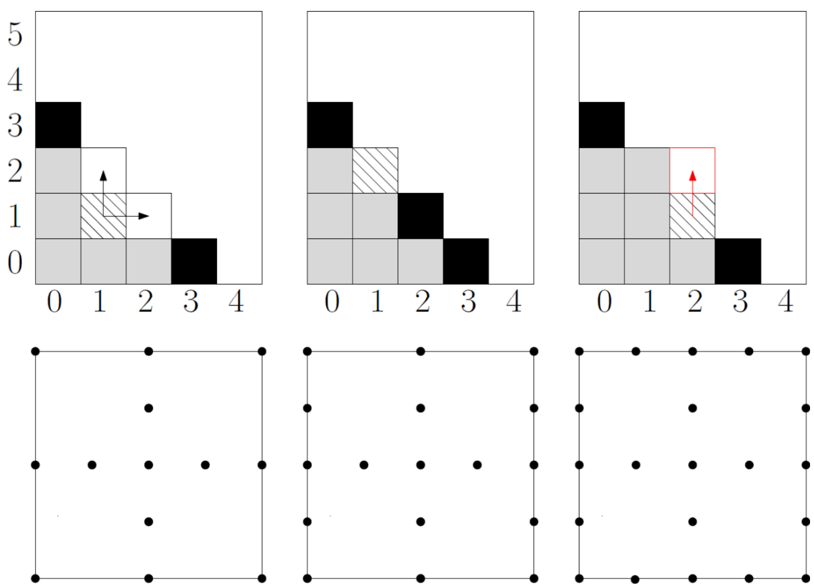
Local Error Estimation with Hierarchical Surpluses

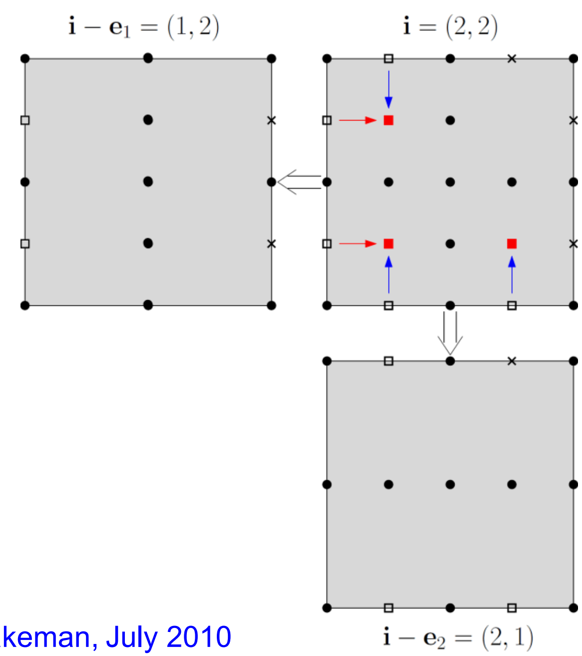
Hierarchical basis:

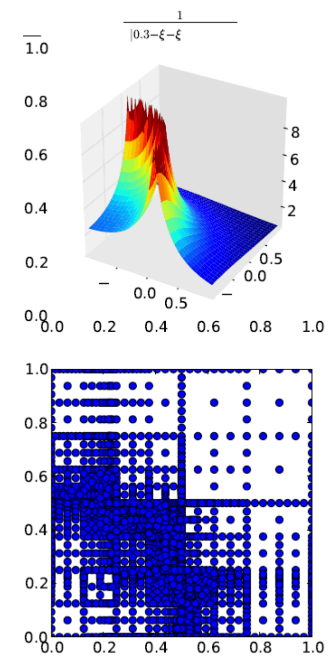
- *Improved precision* in QoI increments
- Surpluses provide error estimates for *local refinement* using local/global hierarchical interpolants
- New error indicators under development that leverage both *value and gradient surpluses*



From X. Ma, 2010







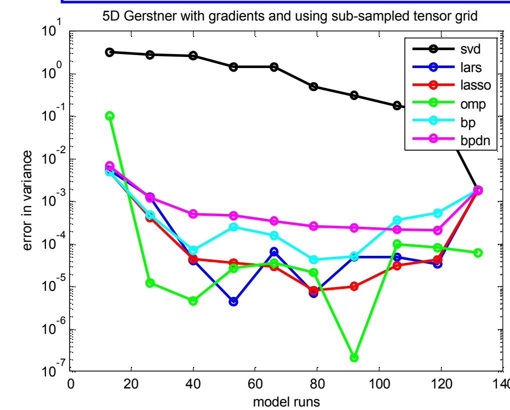
From J. Jakeman, July 2010

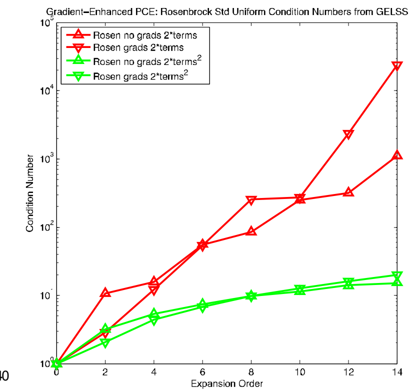
Extend Scalability: (Adjoint) Derivative-Enhancement

PCE:

- **Linear regression including derivatives**
  - **Gradients/Hessians → addtnl. eqns.**
  - **Over-determined: SVD, eq-constrained LS**
  - **Under-determined: compressive sensing**

$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \pi_{0,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) \\ \vdots & \vdots & & \vdots \end{bmatrix} \begin{pmatrix} \vdots \\ \vec{u}^{(m,j)} \\ \vec{u}^{(m+1,j)} \\ \vdots \\ \vec{u}^{(m+n_\xi,j)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \vec{u}_i \\ \frac{\partial \vec{u}_i}{\partial \xi_1} \\ \vdots \\ \frac{\partial \vec{u}_i}{\partial \xi_{n_\xi}} \\ \vdots \end{pmatrix}$$



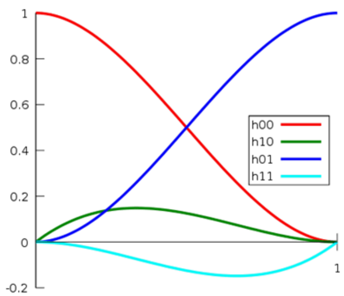


SC:

- **Gradient-enhanced interpolants**
  - **Local: cubic Hermite splines**
  - **Global: Hermite interpolating polynomials**

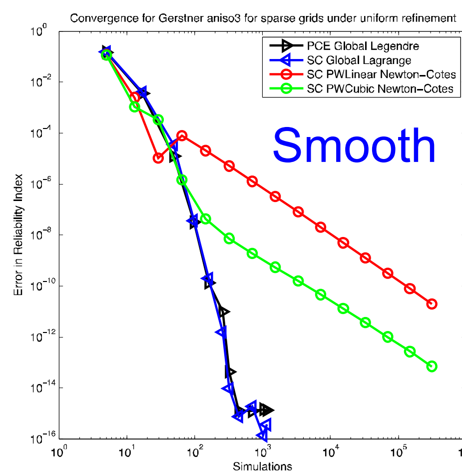
$$f = \sum_{i=1}^{N} f_i H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_1} H_i^{(2)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_2} H_i^{(1)}(x_1) H_i^{(2)}(x_2) H_i^{(1)}(x_3) + \sum_{i=1}^{N} \frac{df_i}{dx_3} H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(2)}(x_3)$$

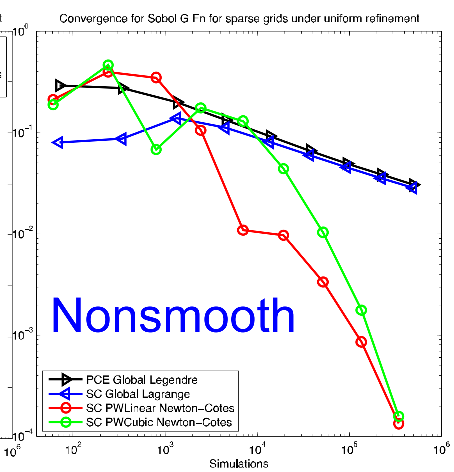
Cubic shape fns: type 1 (value) & type 2 (gradient)



$$\mu = \sum_{i=1}^{N} f_i w_i^{(1)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_1} w_i^{(2)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_2} w_i^{(1)} w_i^{(2)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_3} w_i^{(1)} w_i^{(1)} w_i^{(2)}$$

and similar for higher-order moments





Stochastic Expansions on Unstructured Grids:
Compressive Sensing

$$\begin{bmatrix} f(\mathbf{x}^{(1)}) \\ f(\mathbf{x}^{(2)}) \\ \vdots \\ f(\mathbf{x}^{(N)}) \end{bmatrix} = \begin{bmatrix} 1 & \Phi_2(\mathbf{x}^{(1)}) & \Phi_2(\mathbf{x}^{(1)}) & \dots & \Phi_P(\mathbf{x}^{(1)}) \\ 1 & \Phi_1(\mathbf{x}^{(2)}) & \Phi_2(\mathbf{x}^{(2)}) & \dots & \Phi_P(\mathbf{x}^{(2)}) \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \Phi_1(\mathbf{x}^{(N)}) & \Phi_2(\mathbf{x}^{(N)}) & \dots & \Phi_P(\mathbf{x}^{(N)}) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_P \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_N \end{bmatrix}$$

or in matrix notation

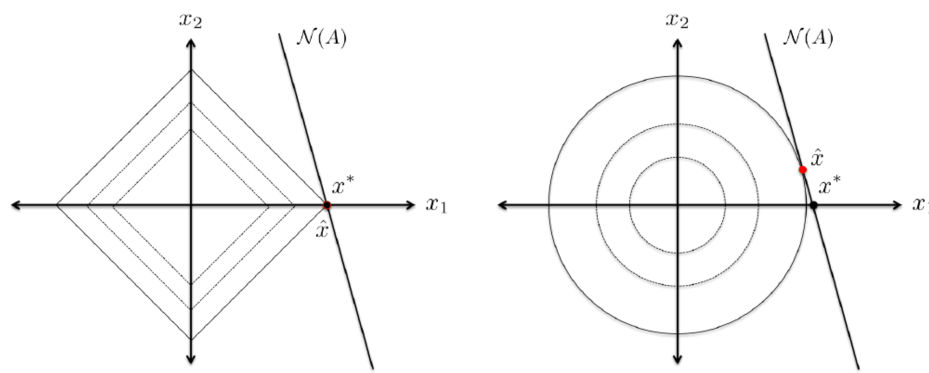
$$\mathbf{b} = \mathbf{Ax} + \varepsilon$$

and find the minimum norm solution

$$\min_{\mathbf{x}} \quad \|\mathbf{Ax} - \mathbf{b}\|_2$$

or (more recently) find a sparse solution

$$\min_{\mathbf{x}} \|\mathbf{x}\|_1 \quad \text{such that} \quad \|\mathbf{Ax} - \mathbf{b}\|_2 \le \varepsilon$$



(a) CS methodology (ℓ_1 objective) (b) Pseudo-inverse (ℓ_2 objective)

BP

$$\mathbf{c} = \arg\min \|\mathbf{c}\|_{\ell^1} \quad \text{such that} \quad \mathbf{\Phi c} = \mathbf{y}$$

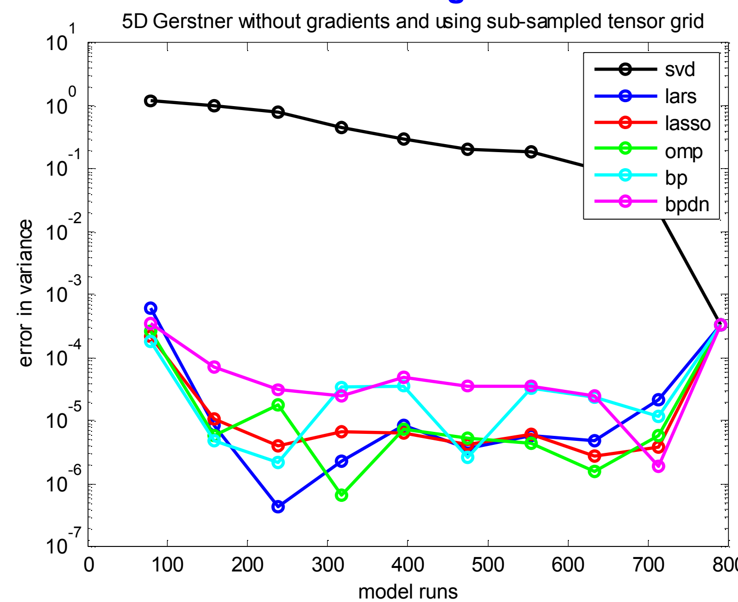
BPDN and OMP

$$\mathbf{c} = \arg\min \|\mathbf{c}\|_{\ell^1} \quad \text{such that} \quad \|\mathbf{\Phi c} - \mathbf{y}\|_{\ell^2} \le \varepsilon$$

LASSO and LARS

$$\mathbf{c} = \arg\min \|\mathbf{\Phi c} - \mathbf{y}\|^2_{\ell^2} \quad \text{such that} \|\mathbf{x}\|_{\ell^1} \le \tau$$

Structured or unstructured grids
Value-based or gradient-enhanced



Adaptive Basis Selection: Compressed Sensing in High Dimensions

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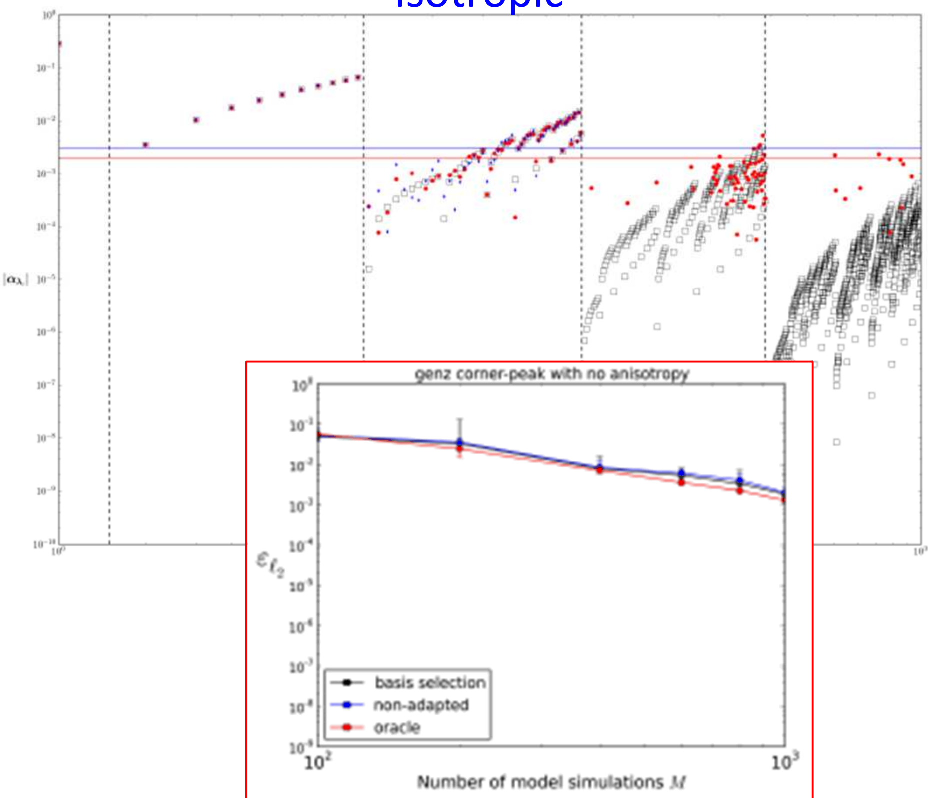
In high dimensions, we may only be able to consider a 2nd or 3rd degree total-order basis

p	3	4	5
$\mathcal{A}^{40}_{3,1}$	$12,341$	$135,751$	$1,221,759$

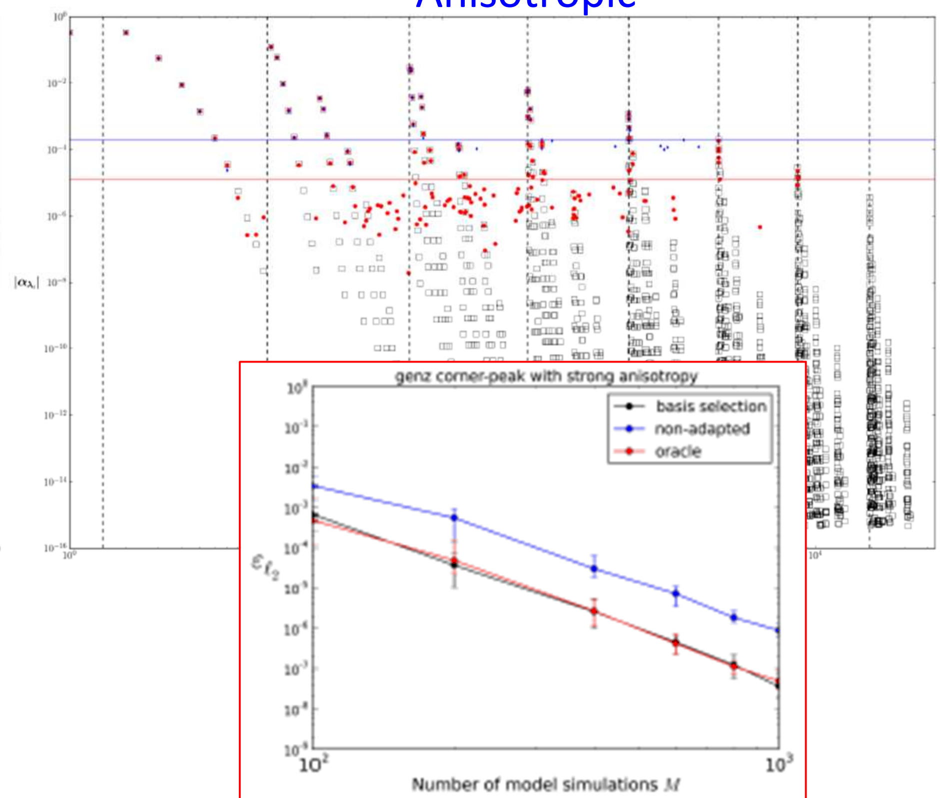
What if the function is anisotropic and important coefficients correspond to p > 3?

We seek algorithms that can adaptively determine an effective basis → ***expanding front***

Isotropic



Anisotropic

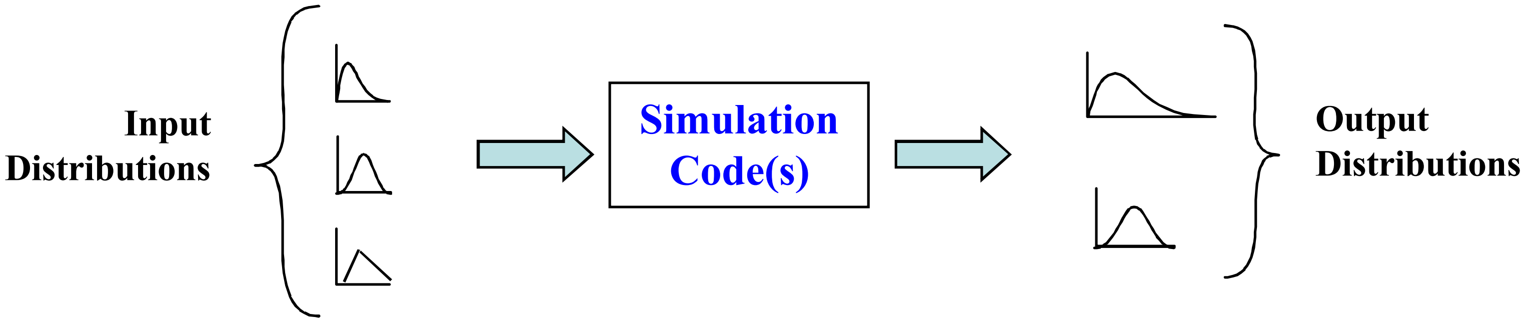


UQ Methods: Epistemic

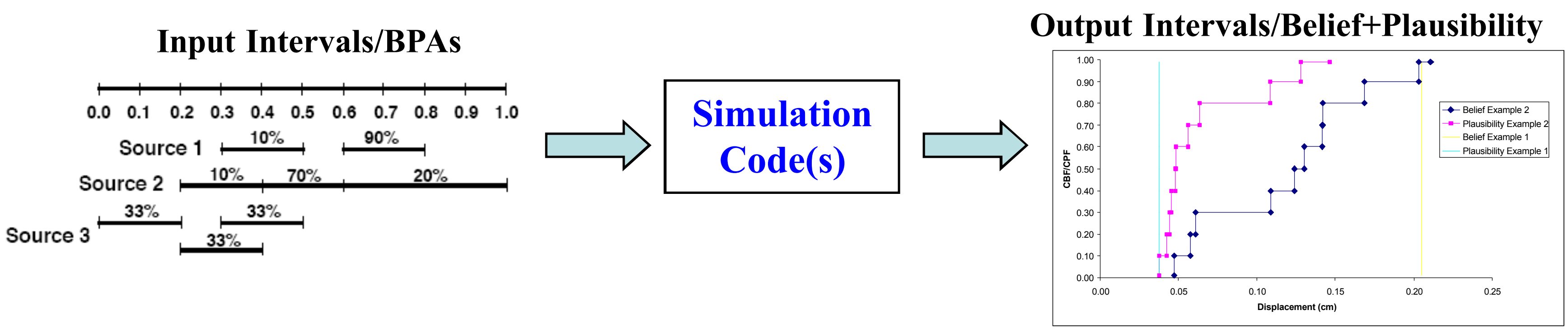
Categorization of Uncertainty

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

- ***Aleatory:*** inherent variability with sufficient data → objective probabilistic models
  - Aka irreducible, type-A, stochastic



- ***Epistemic:*** uncertainty from lack of knowledge → subjective probabilistic & nonprobabilistic models
  - Aka reducible, subjective, type-B, state of knowledge uncertainty
  - Strict interpretation is fully reducible: in perfect state of information, collapses to *constant value*



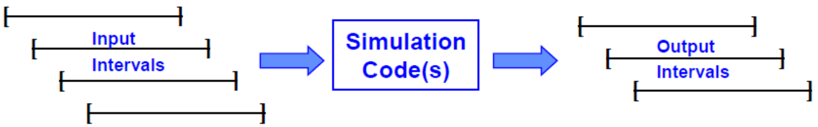
- Bayesian: posterior spectrum from data-dominated to prior-dominated

Epistemic UQ

Epistemic UQ: one does not know enough to specify probability distributions

Sometimes referred to as subjective, reducible, or lack of knowledge uncertainty

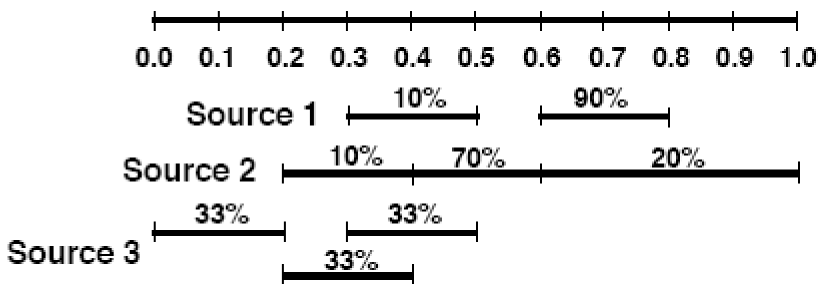
Interval analysis

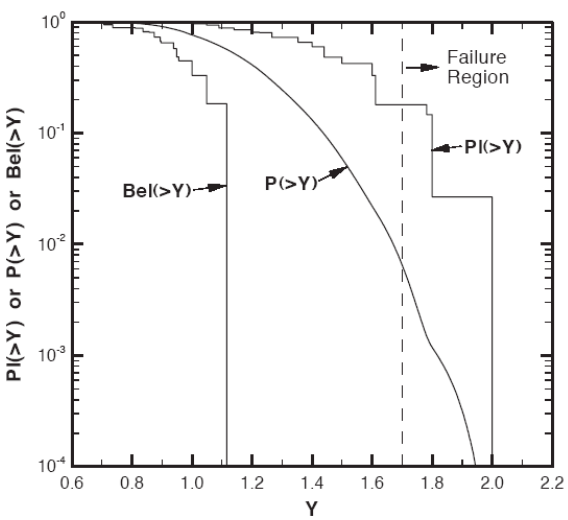


- Propagate input intervals to output intervals
- Intrusive interval methods (operation by operation propagation) have been investigated for several decades, but have not become mainstream (key issue: interval growth)
- Sampling methods (+ surrogate models if expensive evals) are commonly used
- Optimization methods are promising and some variants exploit data reuse

Dempster-Shafer theory of evidence

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





Imprecise probability (p-boxes), Info gap, …

Core UQ Algorithms: strengths, weaknesses, research needs

Sampling (nongradient-based)

- ***Strengths:*** Simple and reliable, convergence rate is dimension-independent
- ***Weaknesses:*** $N^{-1/2}$ convergence → expensive for accurate tail statistics

Local reliability (gradient-based)

- ***Strengths:*** computationally efficient, widely used, scalable to large *n* (w/ efficient/adjoint derivatives)
- ***Weaknesses:*** algorithmic failures for limit states with following features
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. insufficient to resolve probability at MPP

Global reliability (typically nongradient-based)

- ***Strengths:*** handles multimodal and/or highly nonlinear limit states, tailored for efficient probability estimation
- ***Weaknesses:***
  - Conditioning, nonsmoothness → ensemble emulation (recursion, discretization)
  - Scaling to large *n* → adjoint gradient-enhancement, additional refinement bias

Stochastic expansions (typically nongradient-based)

- ***Strengths:*** functional representation, exponential convergence rates for smooth problems, best for moment est.
- ***Weaknesses:***
  - Nonsmoothness → local h-refinement based on hierarchical error estimates
  - Scaling to large *n* → adaptive refinement, adjoint gradient-enhancement, sparsity detection

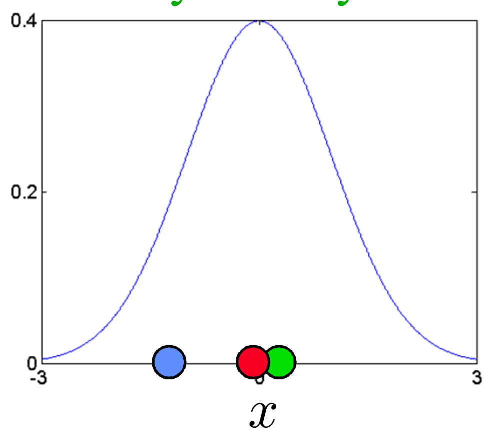
Epistemic methods (typically nongradient-based)

- ***Strengths:*** extrema are point solutions instead of integrated quantities
- ***Weaknesses:*** high degrees of input structure (Dempster-Shafer) require *many* extrema (bridging intervals and distributions breaks down as continuum is approached discretely)

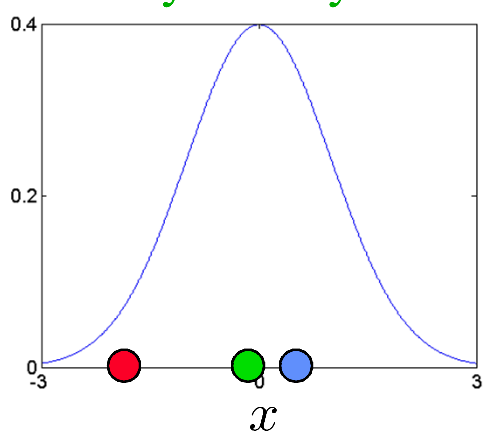
Extra Slides

More General Probabilistic Models are Random in Time and/or Space

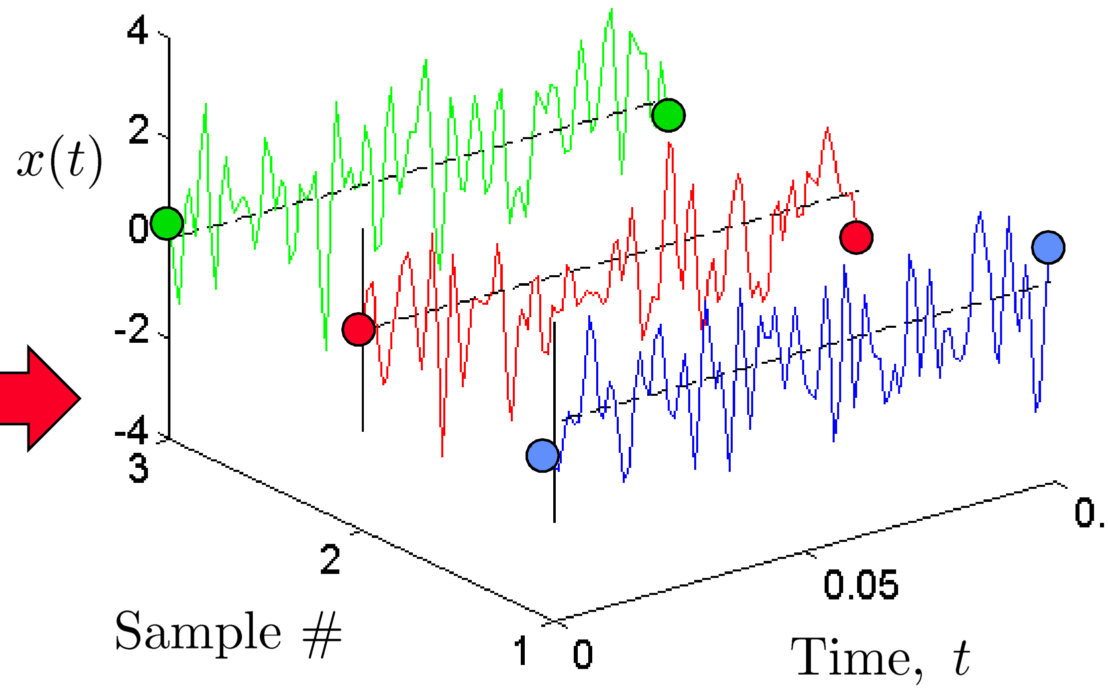
Probability density at $t = 0$



Probability density at $t = 0.1$



3 independent samples of a Gaussian stochastic process



- Stochastic processes can represent time-varying phenomena

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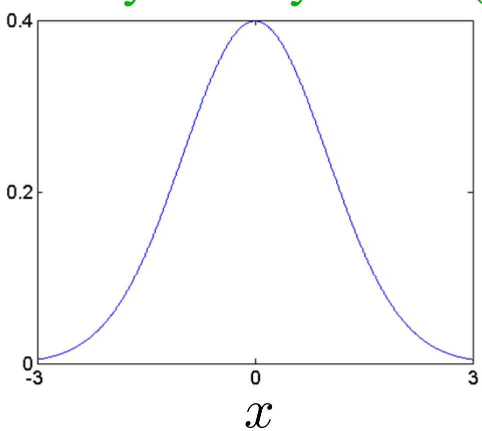
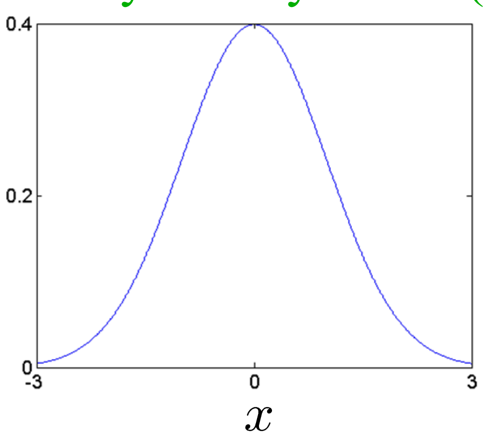
More General Probabilistic Models are Random in Time and/or Space

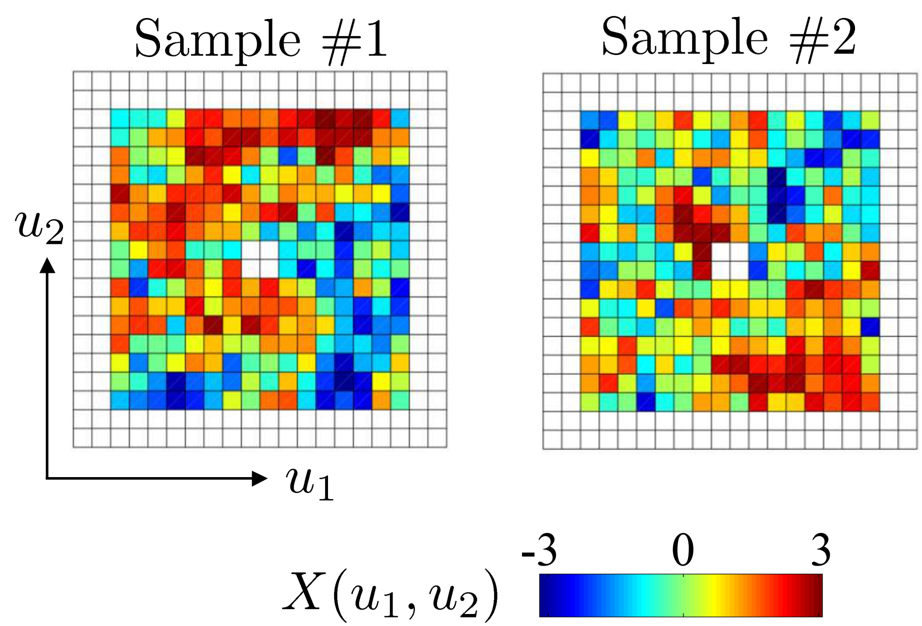
Probability density at $\mathbf{u} = (1,1)^T$



Probability density at $\mathbf{u} = (0,1)^T$



2 independent samples of a Gaussian random field



- Random fields can represent spatially-varying phenomena