Uncertainty Quantification Methods Enabling Credible Simulation

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Optimization and Uncertainty Quantification

(with Michael S. Eldred and Laura P. Swiler)

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Nuclear Engineering / Mathematics Joint Seminar

North Carolina State University

Raleigh, NC

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.

Personal Background

- Ph.D., Computational and Applied Mathematics, NC State
  - mathematics, statistics, computer science, immunology
  - nondeterministic model calibration (HIV)

- SNL, Albuquerque since 2005:
  - went for optimization focus; diversified into UQ
  - mix of algorithm development, production software
  - agent-based disease simulations, power grid optimization, research in mixed integer surrogates

- Algorithms discussed today publicly available in DAKOTA
  - Many science/engineering application customers; their unmet needs drive research and software

- Ongoing work with Hany, INL, ORNL in DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS)

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Outline:
UQ Algorithms for Credible Simulation

GOAL: Demonstrate how a mix of statistics, nonlinear optimization, numerical integration, and surrogate (meta-) modeling enables robust and efficient UQ methods.

- **Motivation for credible simulation (computational models)**
- **Characterizations and propagation of uncertainty**
- **Uncertainty quantification algorithms**
  - **Sampling-based**
  - **Reliability**
  - **Stochastic expansion**
  - **Interval estimation**
- **UQ research challenges and directions**

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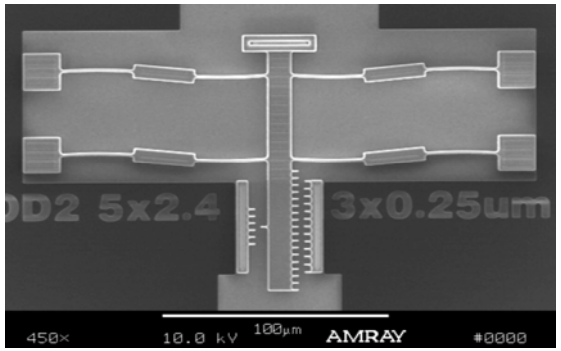
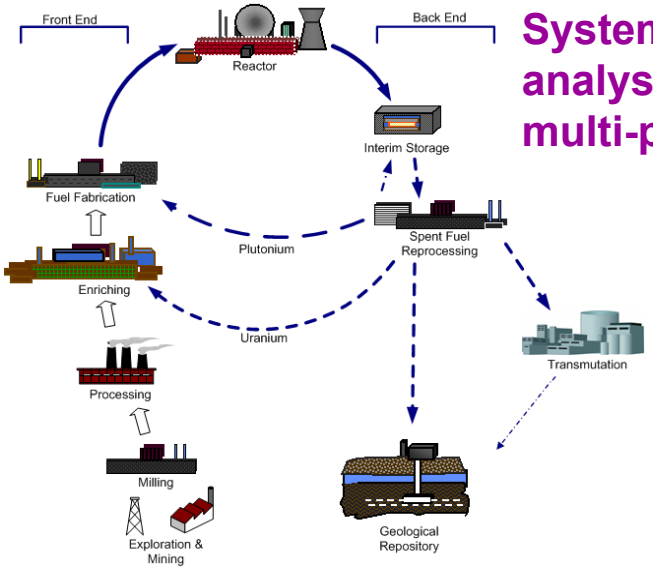
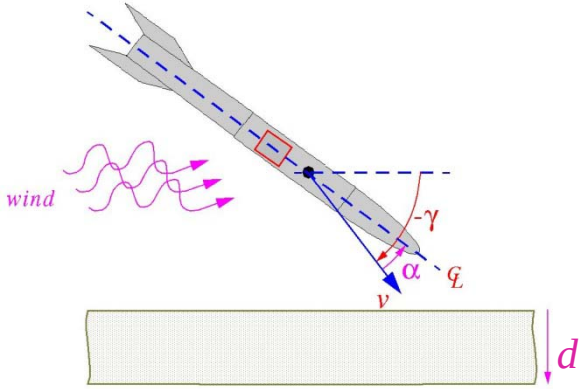
Insight from Computational Simulation



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

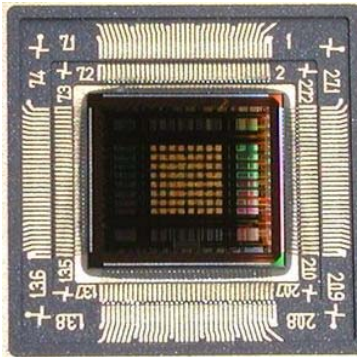


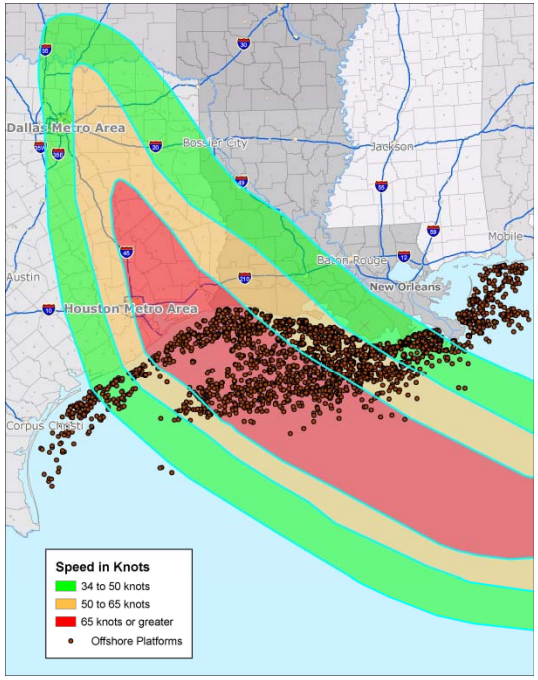
Systems of systems analysis: multi-scale, multi-phenomenon



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

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





Hurricane Katrina: weather, logistics, economics, human behavior

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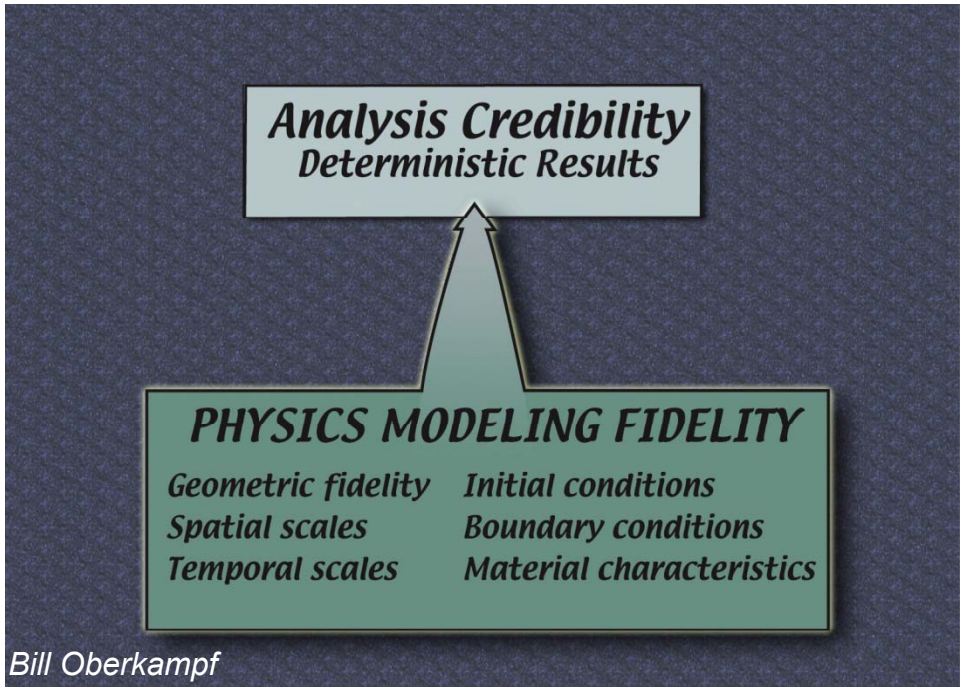
Credible Simulation

- **Historically: primary focus on *modeling fidelity (with enormous investments)***
- **Customers increasingly (should) demand *proof of overall analysis pedigree* in the data and/or extrapolation domain.**



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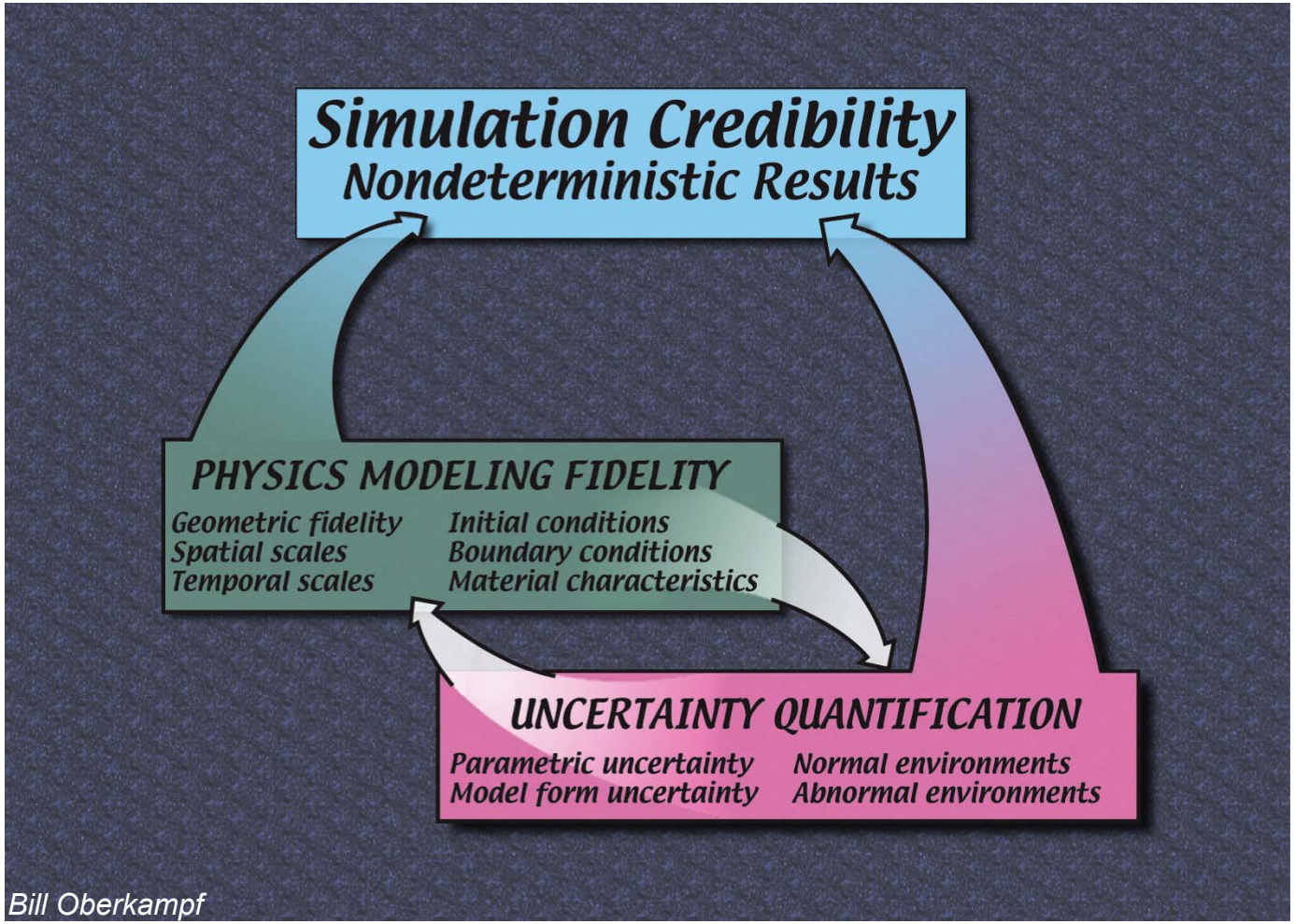
Inclusion of Nondeterministic Element (early 1970's)



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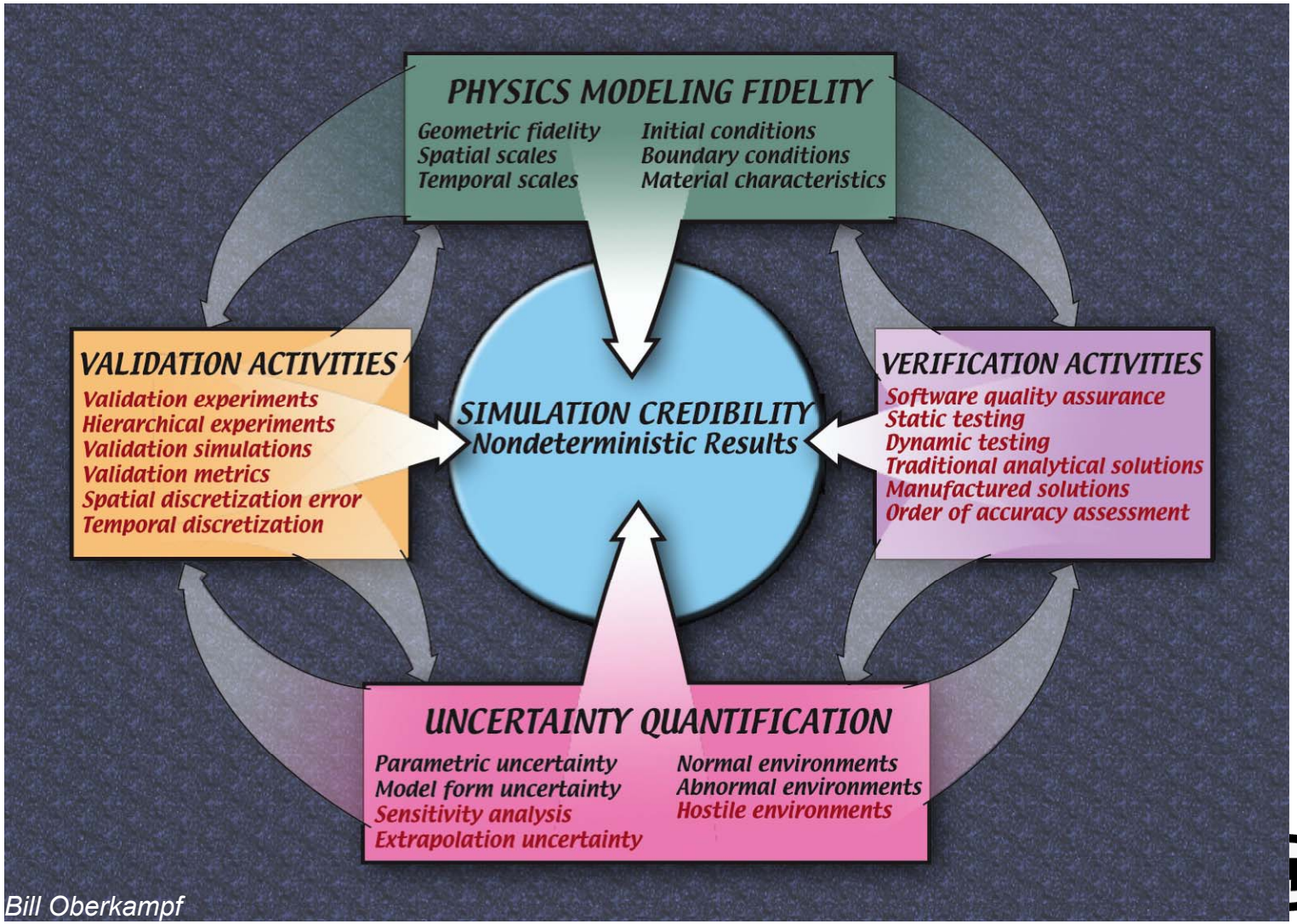
Formal V&V, UQ, and Model Fidelity Support Credible Simulation

Ultimate purpose (arguably): insight, prediction, and risk-informed decision-making → *need credibility for intended application*



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*.**

- **Ideally: code verification → solution verification → validation *then* follow-on optimization/calibration/uncertainty quantification**

Supporting 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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Uncertainties in Simulation and Validation

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

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

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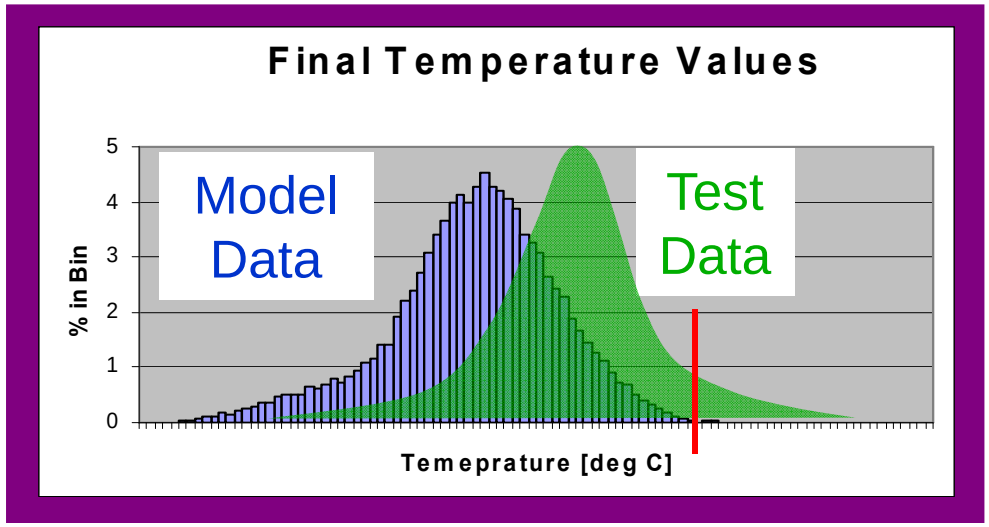
Uncertainty Quantification

- **A single optimal design or nominal performance prediction is often insufficient for**
  - **decision making / trade-off assessment**
  - **quantification of margins and uncertainties (QMU):** ***How close are my uncertainty-aware code predictions to required performance expectations or limits?***

- ***GOAL: risk-informed decisions, based on effects of uncertainty on model output (forward propagation)***

- **Validation:** ***Given the relevant uncertainties,*** **is the science (physics, biology, etc.) model sufficient** ***for the intended application?***



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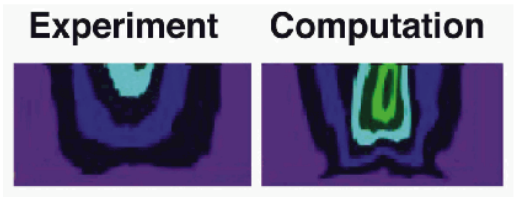
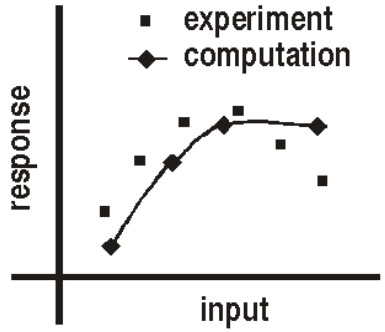
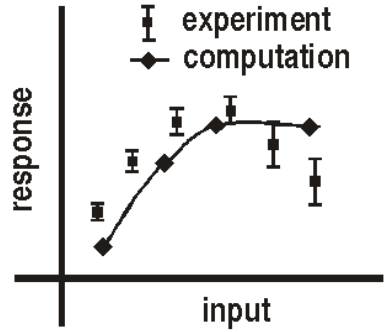
Quantitative Comparison with Experiment: Validation Metrics



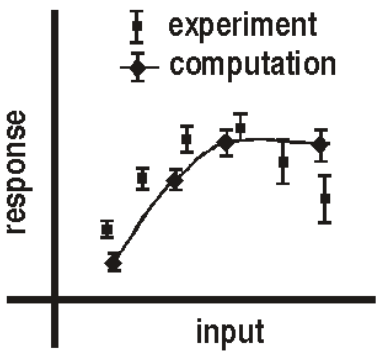
(a) Viewgraph Norm



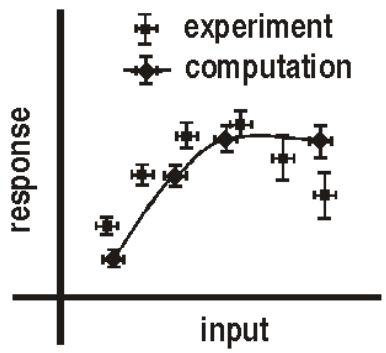
(b) Deterministic



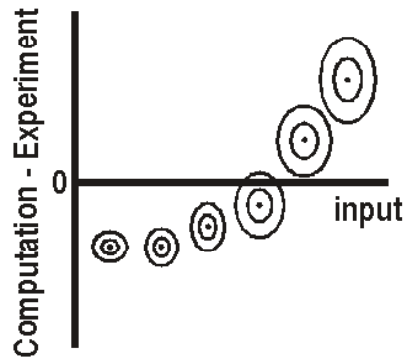
(c) Experimental Uncertainty



(d) Numerical Error



(e) Nondeterministic Computation



(f) Statistical Comparison

Verification to estimate numerical error; uncertainty quantification to assess effect of unknowns or natural variability

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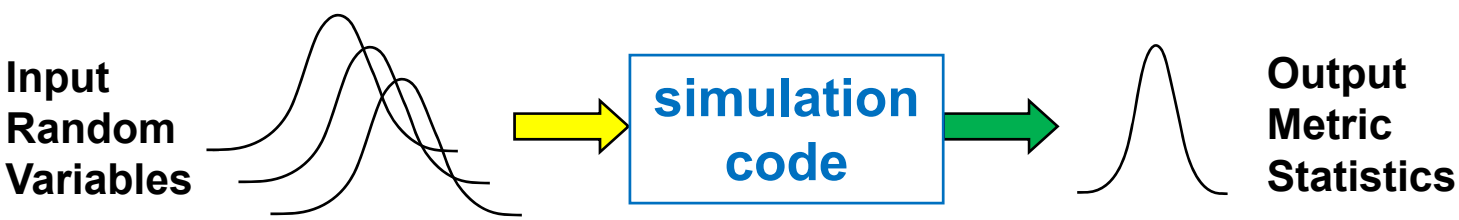
Categories of Uncertainty

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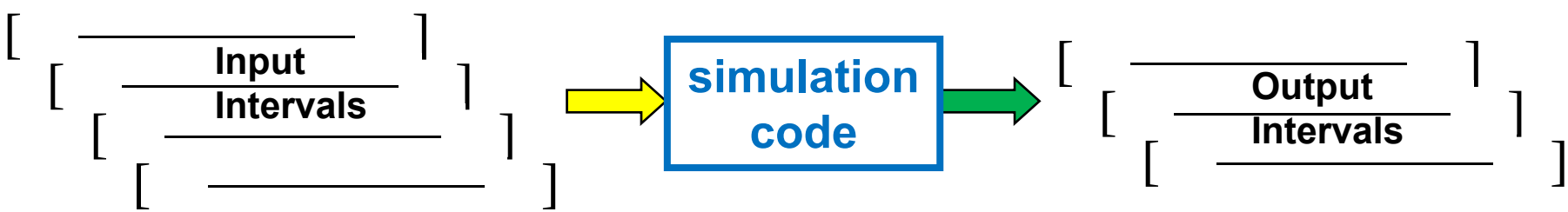
  - **Irreducible uncertainty – can't reduce it by further knowledge**

- **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**



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Uncertainty Quantification

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

Input Variables *u*
(physics parameters, geometry, initial and boundary conditions)

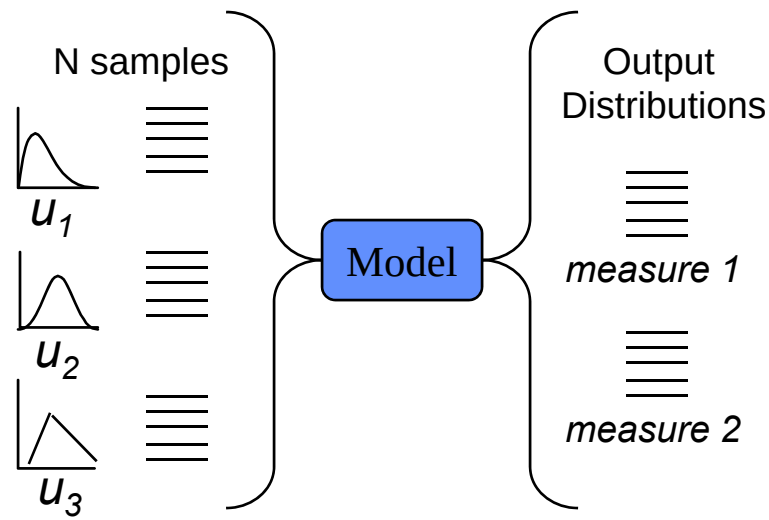
→ **Computational Model** →

Variable Performance Measures *f(u)*

(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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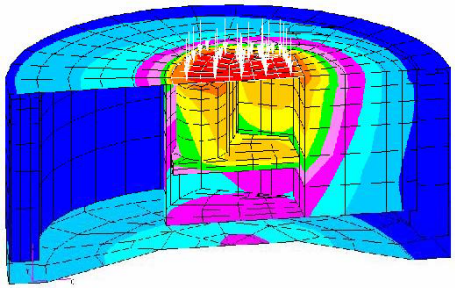
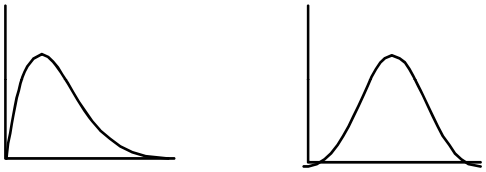
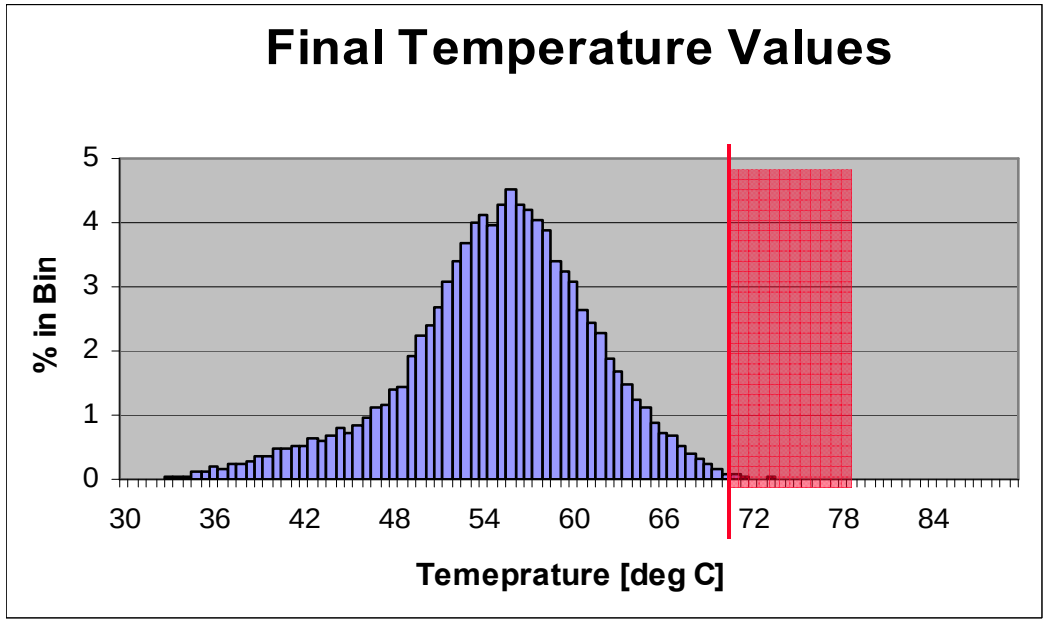
Thermal Uncertainty Quantification

- **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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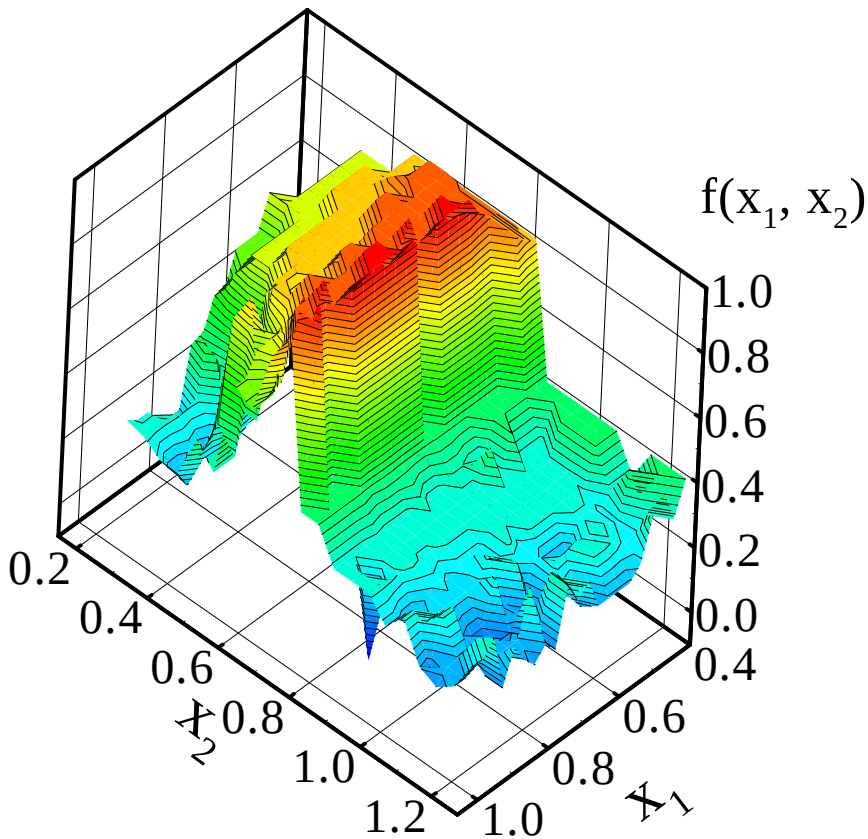
Challenges for Simulation-based UQ

- **Engineering application: propagate variability through a 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**



Is it better to:

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

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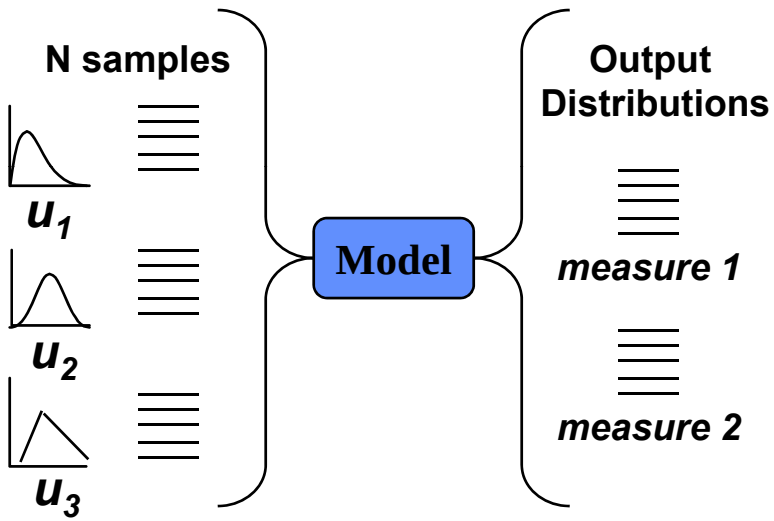
UQ: Sampling Methods

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



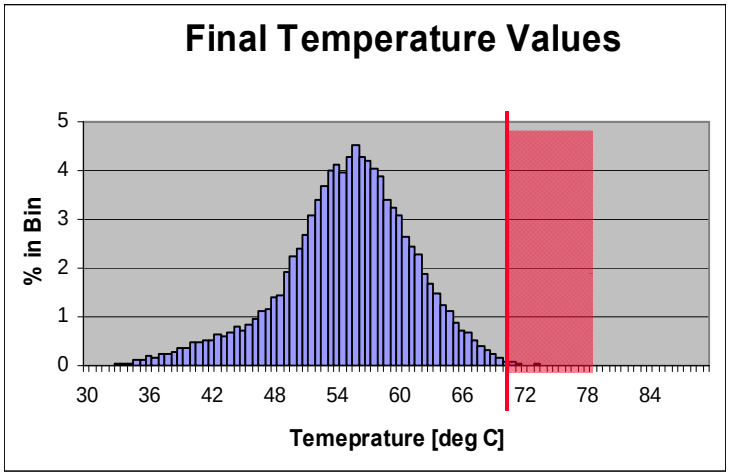
- **sample mean**

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

- **sample variance**

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

- **full PDF(probabilities)**

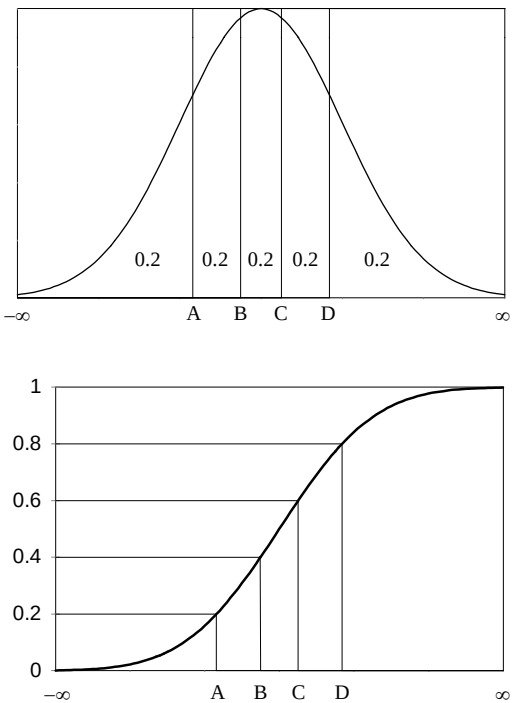


- **Monte Carlo sampling**
- **Quasi-Monte Carlo**
- **Centroidal Voroni Tessalation (CVT)**
- **Latin Hypercube sampling**

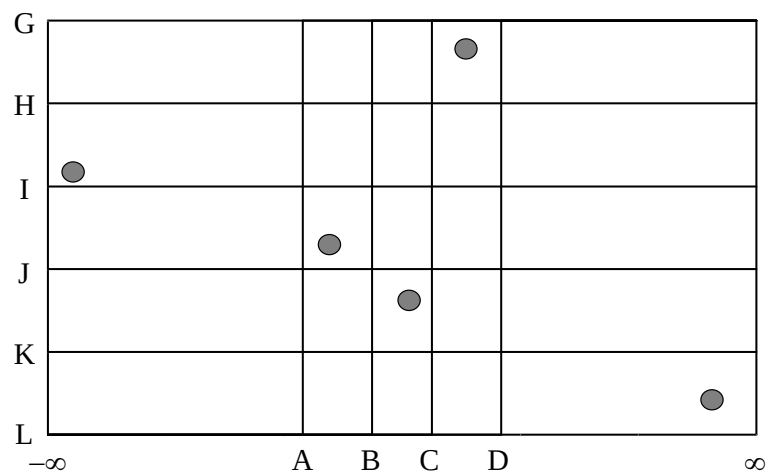
Robust, but slow convergence: $O(N^{-1/2})$

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)

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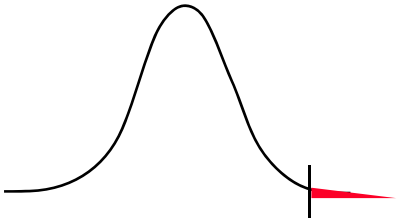
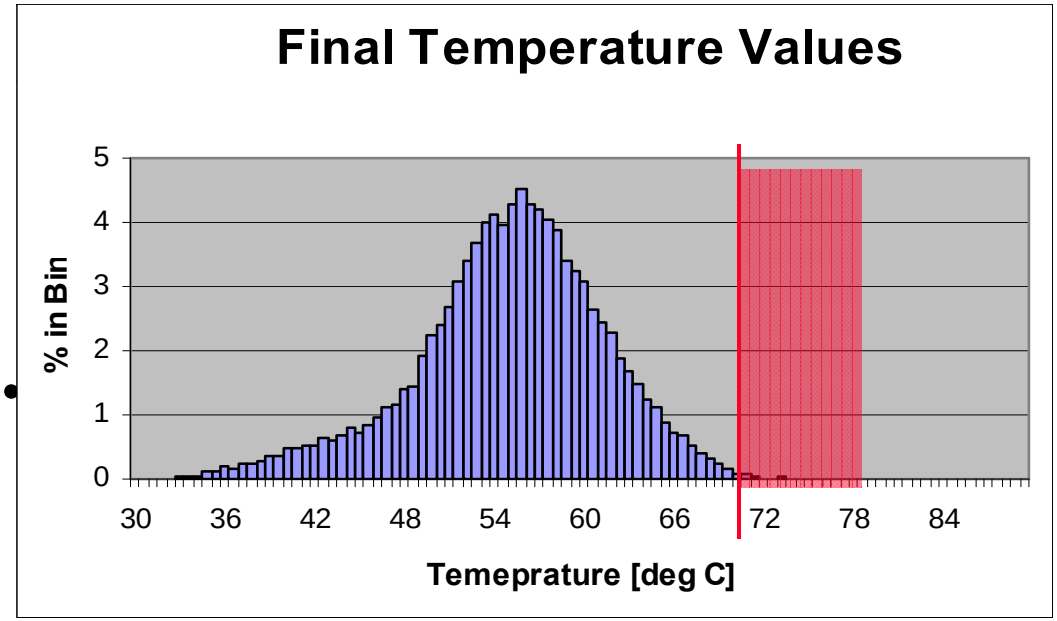
Calculating Probability of Failure

- *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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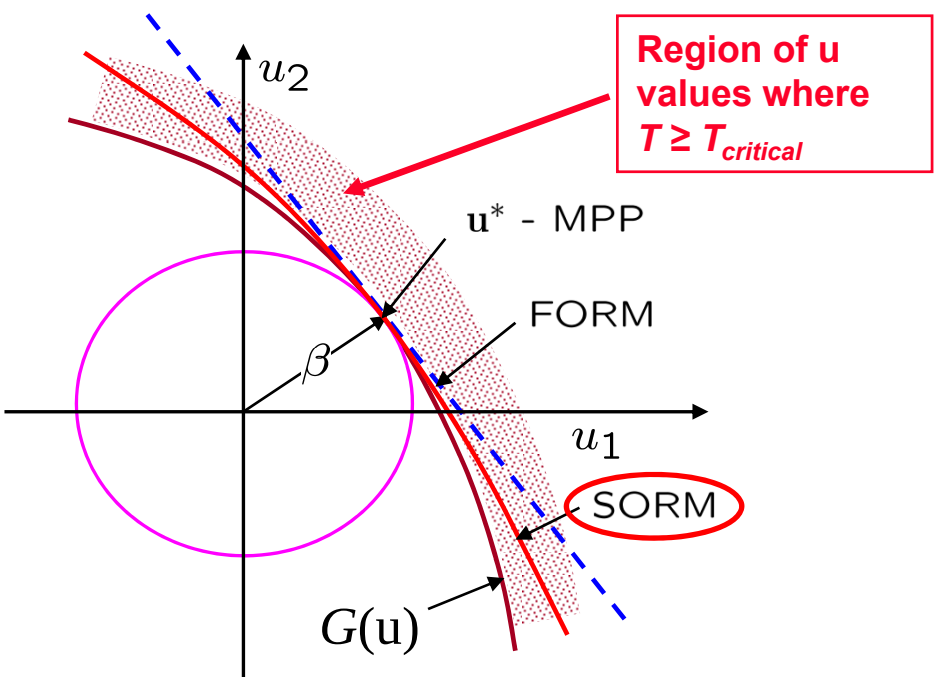
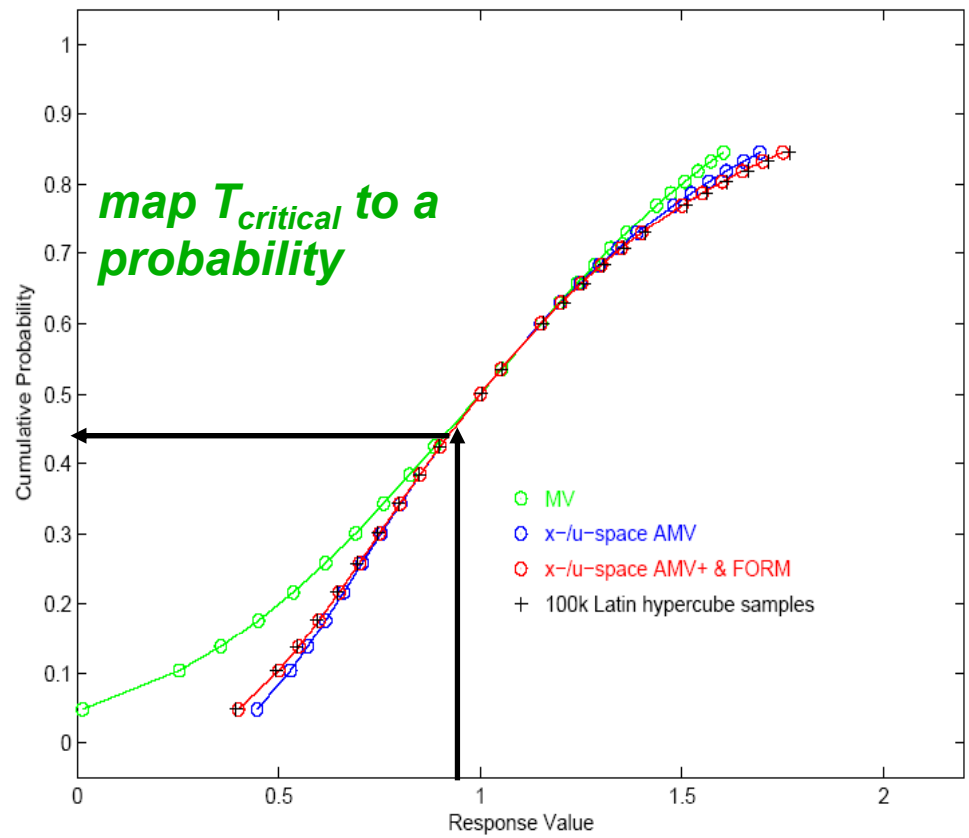
Analytic Reliability: MPP Search

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)

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





Reliability: Algorithmic Variations

Many variations possible to improve efficiency, including in DAKOTA…

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

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

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

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

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

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

$$1^{\text{st}}\text{-order:} \left\{ \begin{array}{lcl} p(g \le z) & = & \Phi(-\beta_{cdf}) \\ p(g > z) & = & \Phi(-\beta_{ccdf}) \end{array} \right. \qquad 2^{\text{nd}}\text{-order:} \left\{ p = \Phi(-\beta) \underbrace{\prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta\kappa_i}}}_{\text{curvature correction}} \right.$$

- **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**

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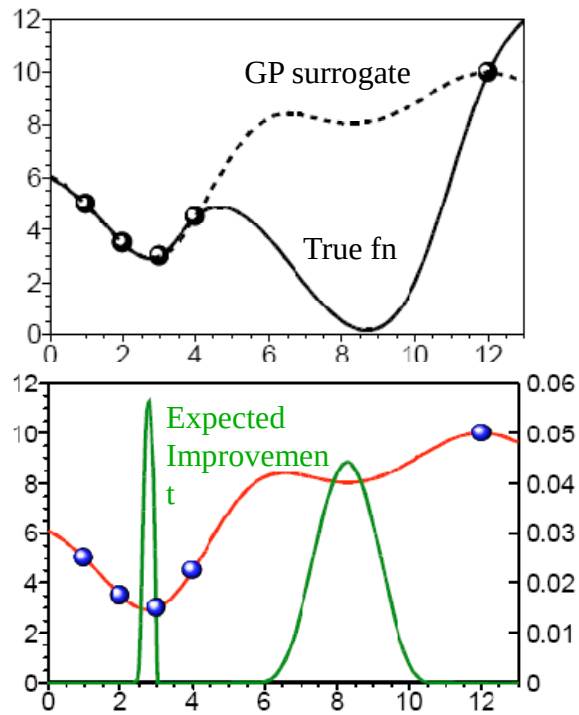
Efficient Global Reliability Analysis

- **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 EGO: expected improvement is large near promising minima, or in regions of high uncertainty**



From Jones, Schonlau, Welch, 1998

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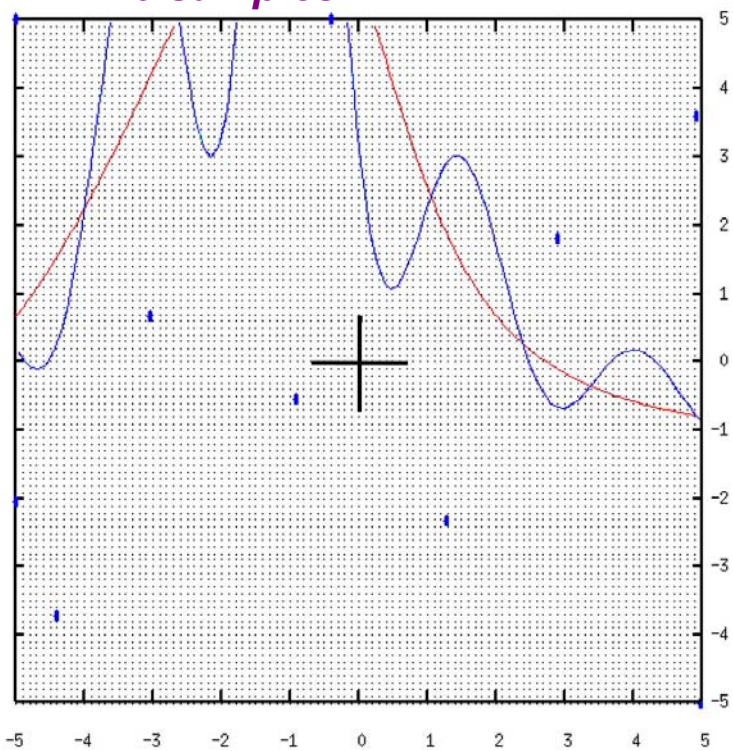
Efficient Global Reliability Analysis

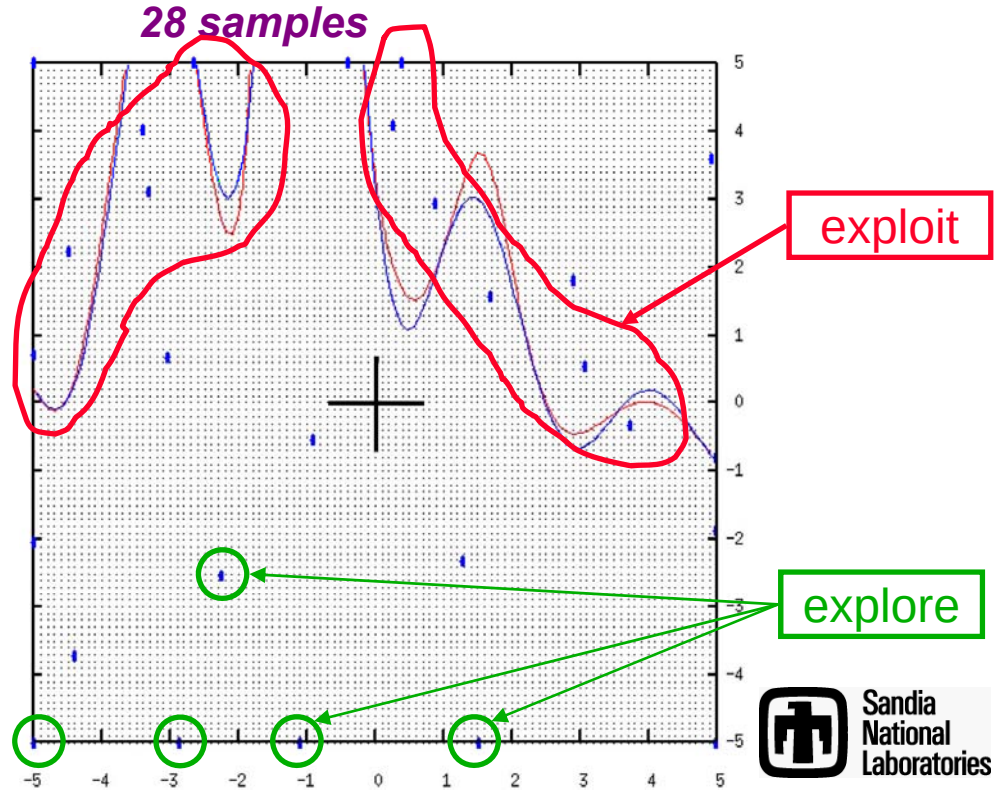
- Apply an EGO-like method to the equality-constrained optimization problem
- In EGRA, an expected feasibility function balances exploration with local search near the failure boundary to refine the GP
- Cost competitive with best MPP search methods, yet better probability of failure estimates

Gaussian process model of reliability limit state with

10 samples



28 samples



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Stochastic Expansions

- Create 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. $$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi})$$ **using**

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

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

- **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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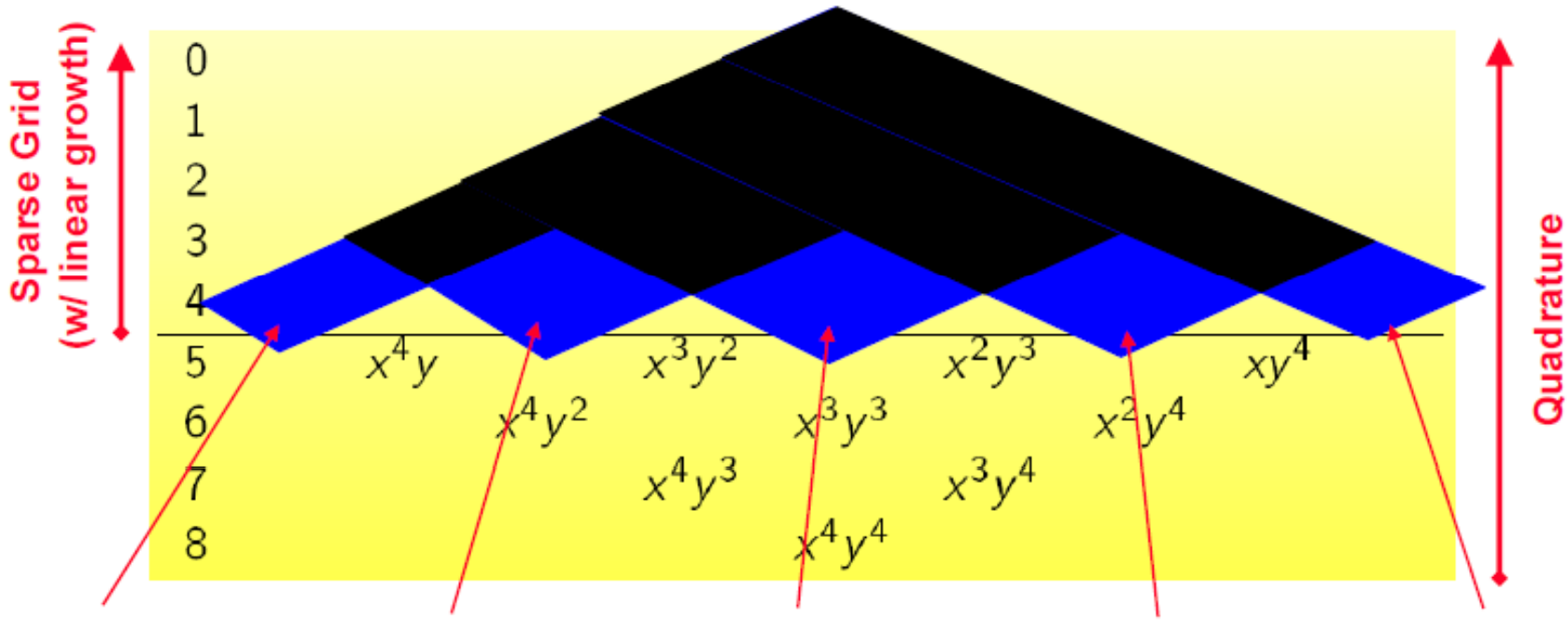
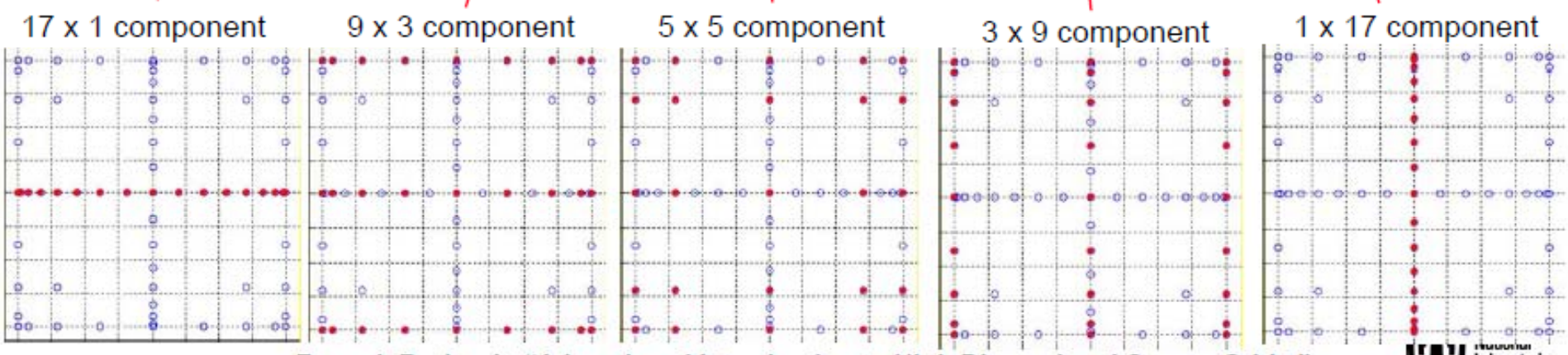
Efficient Integration

Key difference between quadrature & sparse grids: **polynomial order coverage**





From J. Burkardt, "A Low Level Introduction to High Dimensional Sparse Grids."

Stochastic Collocation (based on Lagrange interpolation)

$$L_i = \prod_{\substack{j=1 \\ j \neq i}}^{m} \frac{x - x_j}{x_i - x_j}$$

Instead of estimating coeffs for known basis fns, form interpolants for known coefficients

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

$$R = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n}\right)$$

Form sparse interpolant using S of tensor products (same as forming sparse grid)

Key is use of same Gauss points/weights from the orthogonal polynomials for specified input PDFs → same exponential convergence rates

Simpler than PCE, and:

- **Adapts to integration approach / collocation pt set: doesn't over-/under-integrate a (nonsynchronized) expansion**
- **Estimating moments of any order is easy: $E[R^k] = S\, r^k_j\, w_j$**

$$\mu_R = \sum_{j=1}^{N_p} r_j w_j$$

$$\sigma_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2$$

Disadvantages relative to PCE:

- **Requires structured data sets: quadrature/sparse grid (cubature?), no random sets**
- **Expansion variance not guaranteed positive, no analytic VBD**

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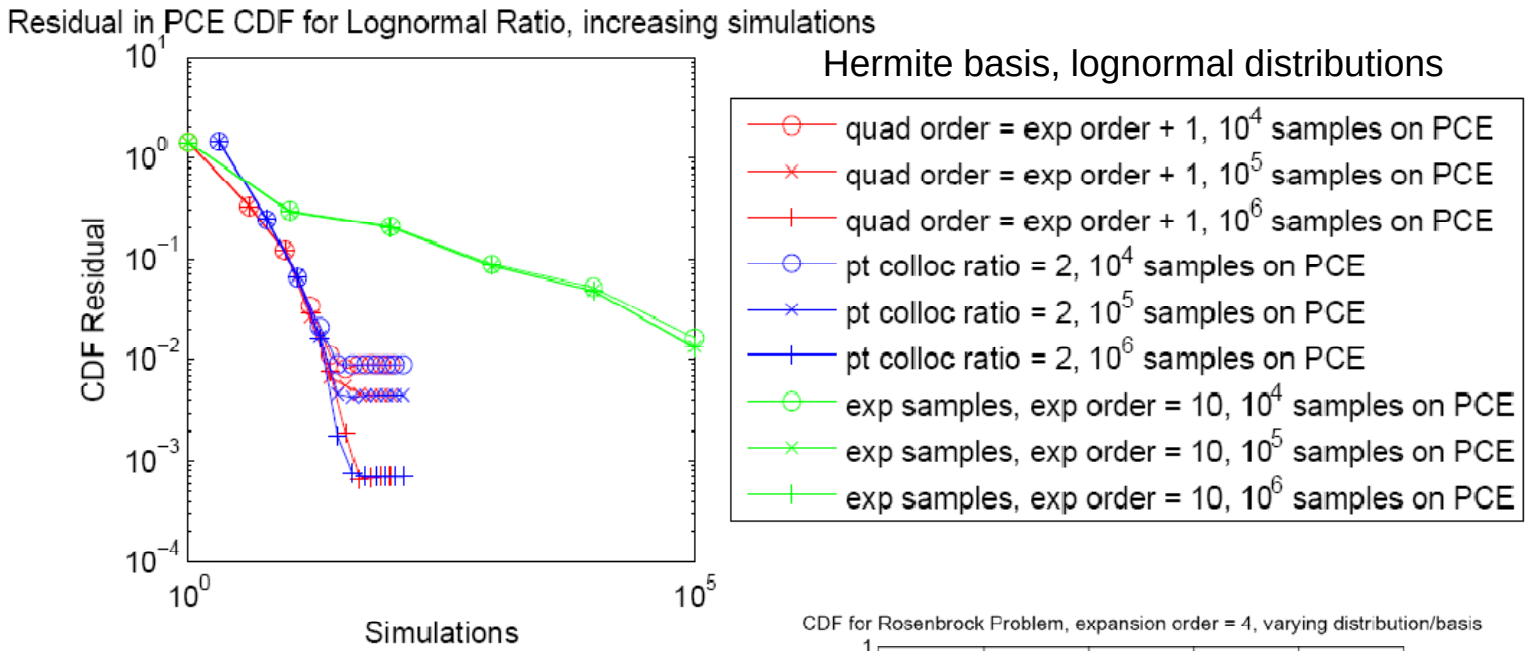
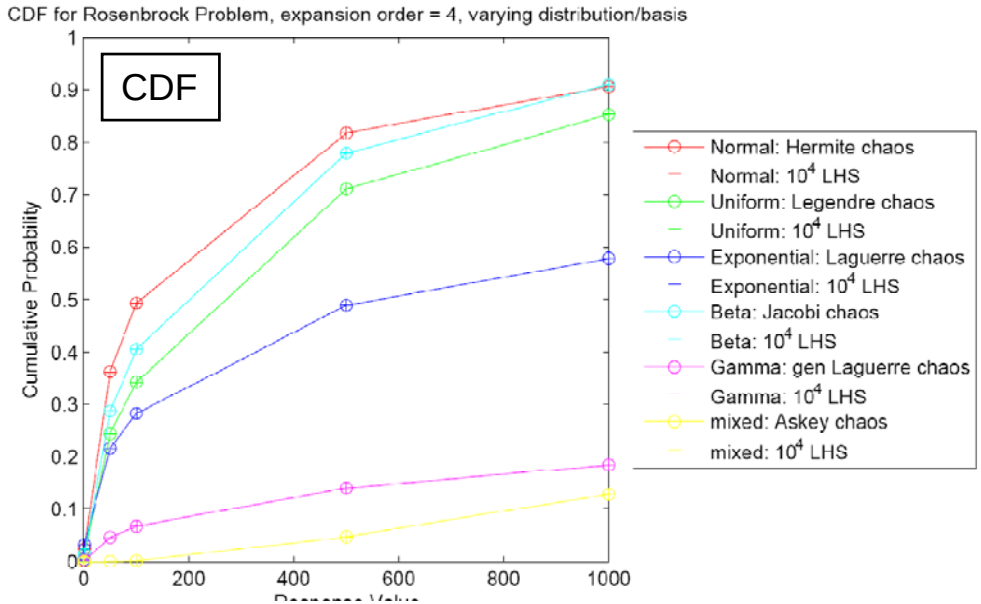
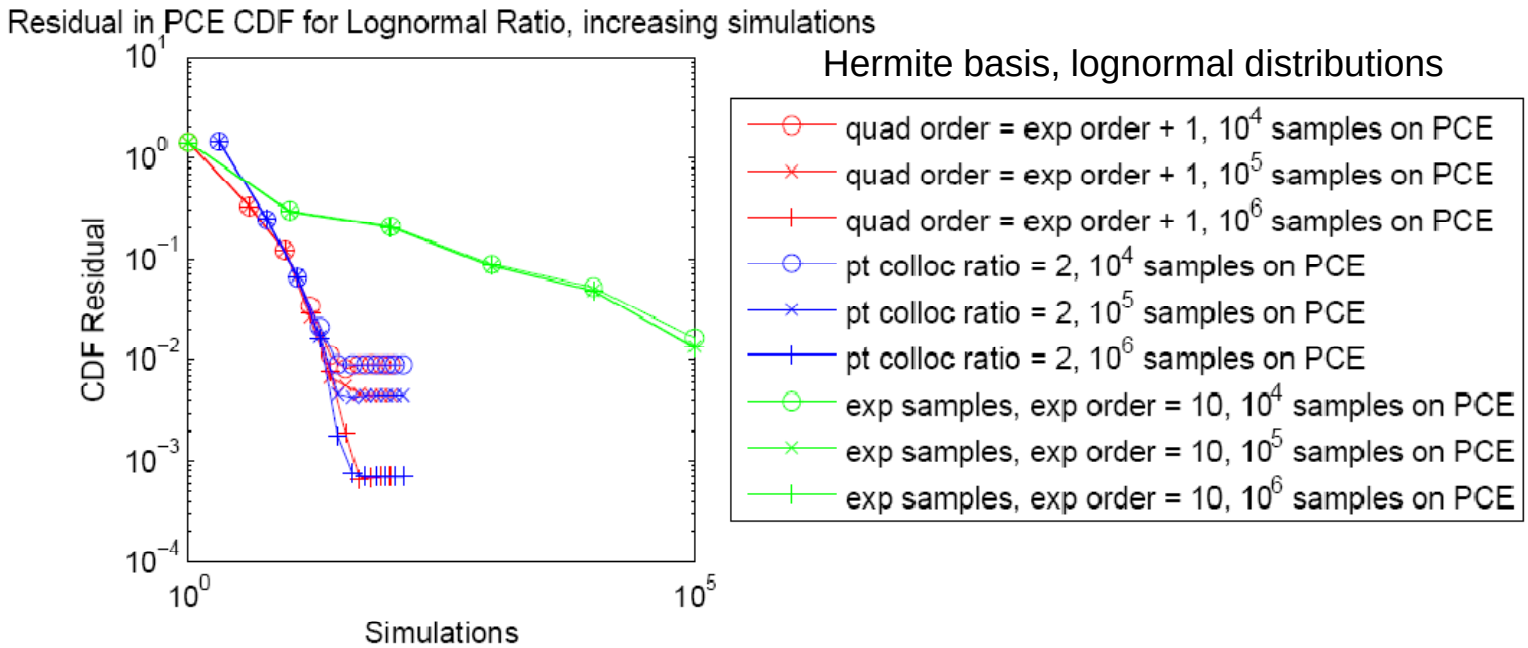
Fast Convergence





Fast Convergence



CDF

Strengths: **functional representation, exponential convergence rates**

Issues:

- **Discontinuity → Gibbs phenomena**
- **Singularity → divergence in moments**
- **Scaling to large *n* → exponential growth in simulation reqmts**

Research:

- **Pade approximation**
- **Basis enrichment / discretization (→ local basis functions)**
- **Dimension adaptive methods**

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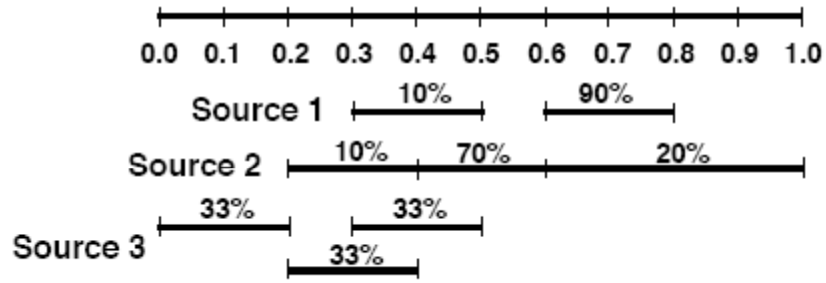
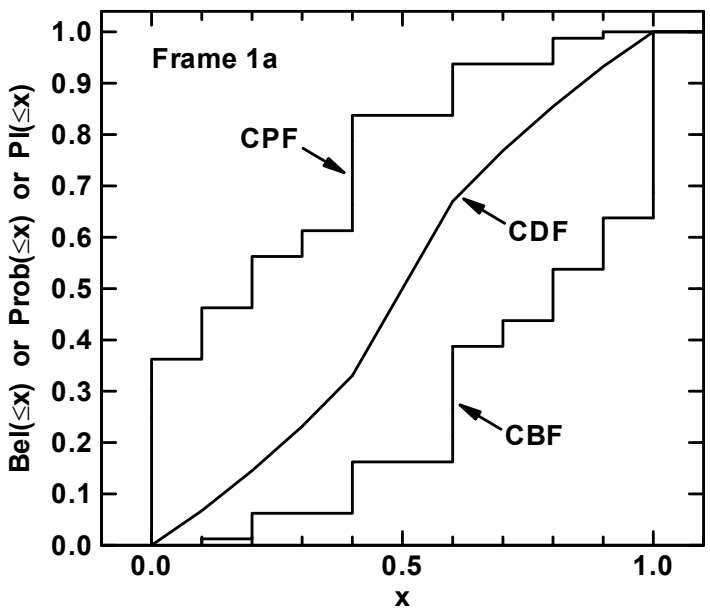
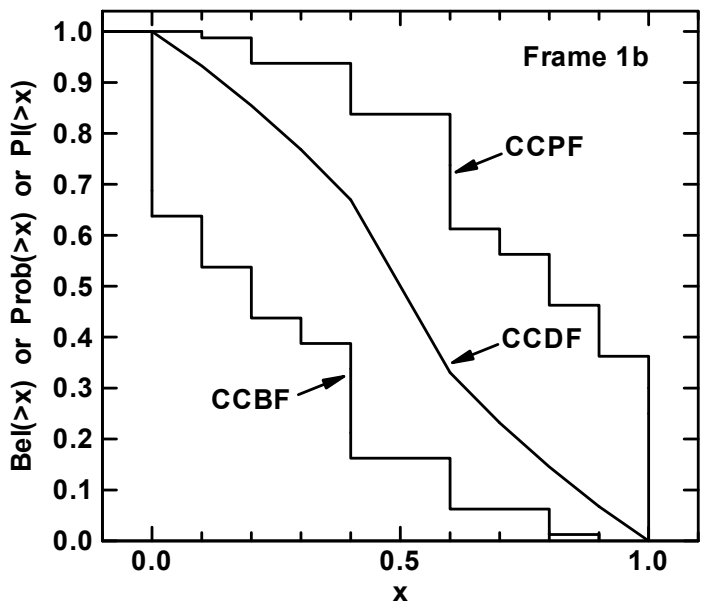
Dempster-Shafer Theory

Intervals on the inputs are propagated to calculate



- **Belief:** a lower bound on a probability value that is consistent with the evidence
- **Plausibility:** an upper bound on a probability value that is consistent with the evidence.





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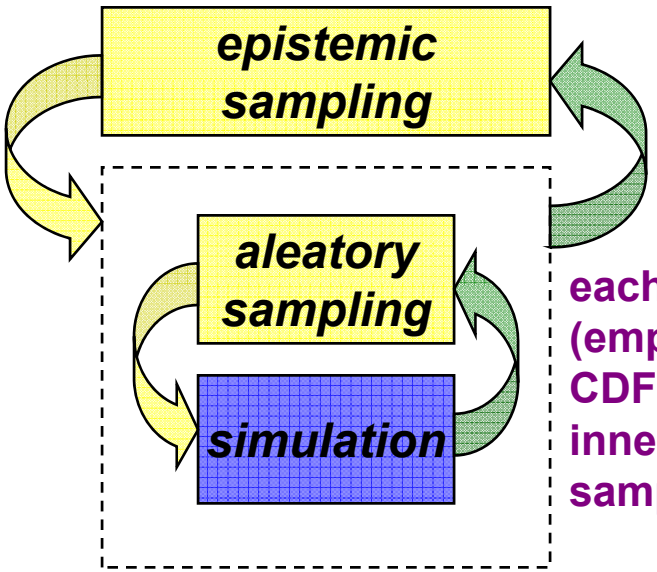
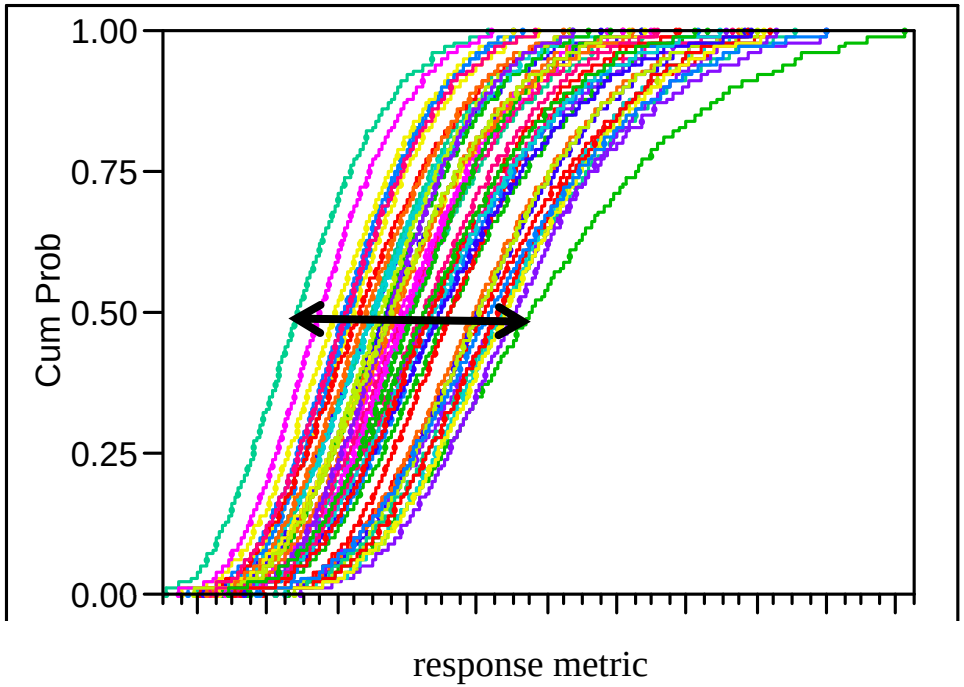
"Second-Order" Probability

- Nested sampling technique which combines epistemic and aleatory uncertainty, e.g., UQ with bounds on the mean of a normal distribution
- Frequently used in UQ studies and regulatory analyses (e.g. WIPP)
- For each outer loop sample of epistemic (interval) variables, run an inner loop UQ study over aleatory (probability) variables; *potentially costly*

50 outer loop samples
→ 50 CDF traces



each discrete (empirical) CDF: 100 inner loop samples



"Envelope" of CDF traces represents response epistemic uncertainty

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New Interval Estimation Approach

- **Outer loop:** determine interval on a moment (e.g., mean or variance)
  - global optimization problem: find max/min of statistic of interest, given bound constrained interval variables
  - use EGO to solve 2 optimization problems with essentially one Gaussian process surrogate

- **Inner loop:** Use stochastic expansion methods (PCE) to determine the CDFs or moments with respect to the aleatory variables

$$\min_{u_E} \; f_{STAT}(u_A \mid u_E)$$
$$u_{LB} \le u_E \le u_{UB}$$
$$u_A \sim F(u_A)$$

$$\max_{u_E} \; f_{STAT}(u_A \mid u_E)$$
$$u_{LB} \le u_E \le u_{UB}$$
$$u_A \sim F(u_A)$$

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Sandia Research Interests

GOAL: Advanced efficient, robust, accurate UQ methods for validation, extrapolation, *risk-informed decisions*

- **Efficient, adaptive polynomial chaos techniques**
- **UQ and surrogate approaches for mixed-integer, higher-order moments, tail statistics**
- **Multi-level (system and hierachical) UQ**
- **How to allocate margin across a system**
- **Stochastic processes and random fields**
- **Epistemic UQ approaches and alternative frames**
- **Adaptive UQ in multi-fidelity/hierarchical contexts**

Thank you for your attention!

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EXTRA SLIDES

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Code Verification: ASC Software Quality Plan Practices

Verification: "Are we solving the equations correctly?"

Project Management
- Integrated Teaming
- Graded Level of Formality
- Measurement & Analysis
- Requirements Development and Management
- Risk Management
- Project Planning & Oversight

Software Engineering
- Technical Solution
- Software Development
- Configuration Management
- Product Integration
- Deployment and Lifecycle Support

Software Verification
- Verification Plan
- Technical Reviews
- Testing (incl. regression)
- Acceptance Criteria

Training
- Team Professional development
- Track Training: prove team qualification

- **Implementation of software quality practices is tailored to the stated level of risk (formality) in using the particular code**
- **Software projects are routinely assessed to these practices (internal and external review)**

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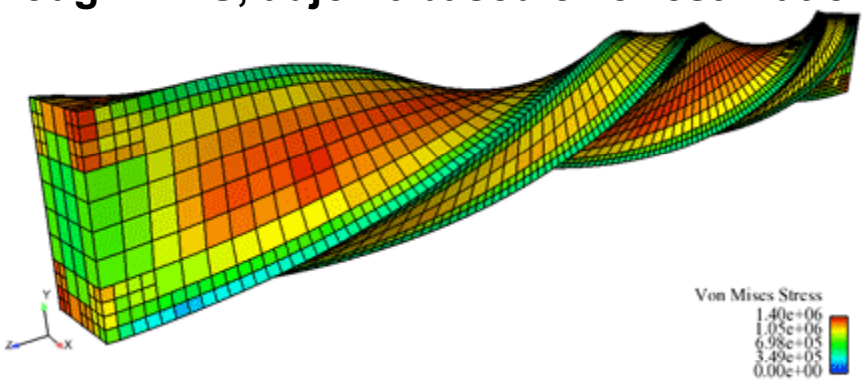
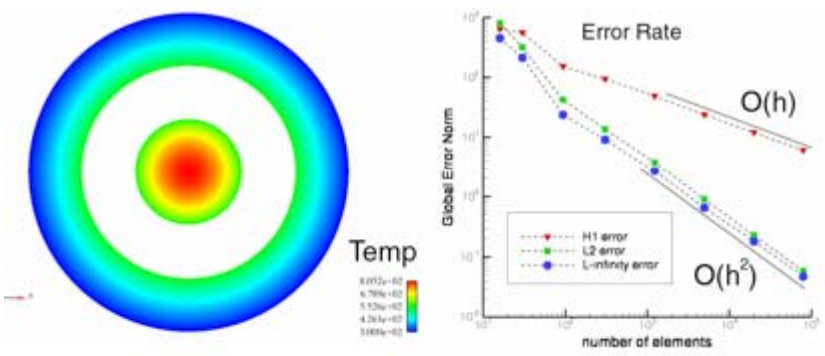
Solution Verification:
Is the solution behaving as expected?

Verification: "Are we solving the equations correctly?"

- **Do we correctly solve problems with analytic and/or known solutions?**
- **Do we realize the expected order of accuracy in space and/or time?**
- **Relevant methods:**
  - **Method of manufactured solutions (MMS)**
  - **Grid convergence studies / Richardson extrapolation**
  - **SIERRA Encore: Online verification through MMS, adjoint-based error estimation, and adaptivity:**

Application of the new error estimator in Encore to a large rotation 3D structural torsion problem solved using the SIERRA Mechanics code Adagio. The mesh adaptivity is driven by the errors in the displacement gradients.





A verification problem for coupled conduction and thermal radiation using the Encore/MMS capability in SIERRA Mechanics. Temperature contours are shown on the left, and convergence rates are shown on the right. Encore has quantified that the simulation has the expected accuracy, providing evidence that the numerical algorithms have been implemented correctly.

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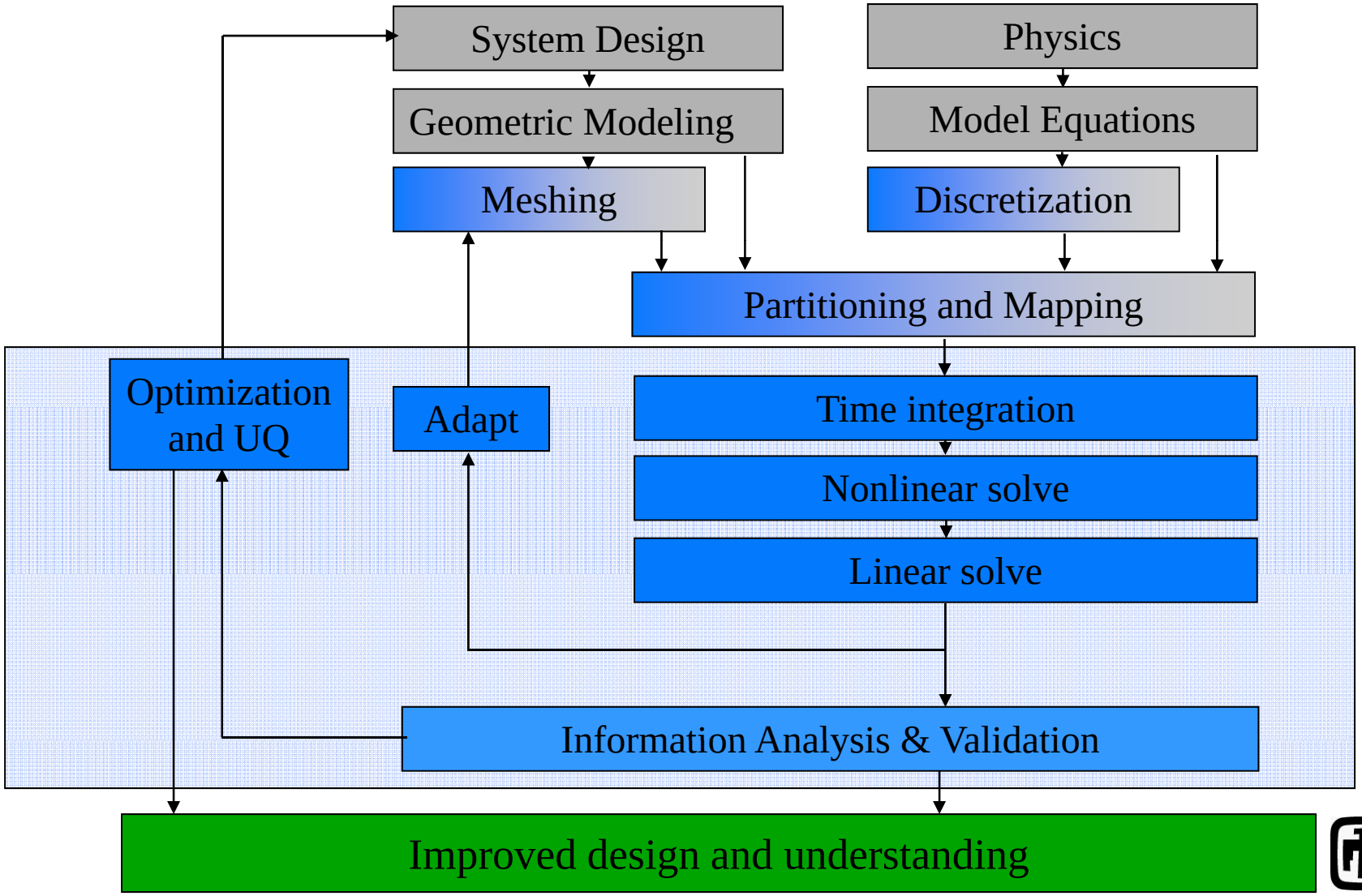
Algorithms for Computational Modeling & Simulation

Are you sure you don't need verification?!



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