Managing Complexity in Simulation-Based Uncertainty Quantification

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• Research group goal: general-purpose uncertainty quantification (UQ) algorithms and software applicable to expensive or otherwise challenging computational models.

• Motivation for uncertainty quantification (UQ); characterizing uncertainties
• Accessible introduction to UQ methods, challenges, some advances
• Challenging environments: coupled multi-physics, random fields, etc.
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
V&V, UQ, and Model Fidelity Support Credible Simulation

Insight, prediction, and risk-informed decision-making require credibility for intended application.

- **PHYSICS MODELING FIDELITY**
  - Geometric fidelity
  - Spatial scales
  - Temporal scales
  - Initial conditions
  - Boundary conditions
  - Material characteristics

- **VALIDATION ACTIVITIES**
  - Validation experiments
  - Hierarchical experiments
  - Validation simulations
  - Validation metrics
  - Spatial discretization error
  - Temporal discretization

- **SIMULATION CREDIBILITY**
  - Nondeterministic Results

- **VERIFICATION ACTIVITIES**
  - Software quality assurance
  - Static testing
  - Dynamic testing
  - Traditional analytical solutions
  - Manufactured solutions
  - Order of accuracy assessment

- **UNCERTAINTY QUANTIFICATION**
  - Parametric uncertainty
  - Model form uncertainty
  - Sensitivity analysis
  - Extrapolation uncertainty
  - Normal environments
  - Abnormal environments
  - Hostile environments

Bill Oberkampf
A few uncertainties affecting computational model output/results:

- physics/science parameters
- statistical variation, inherent randomness
- model form / accuracy
- material properties
- manufacturing quality
- operating environment, interference
- initial, boundary conditions; forcing
- geometry / structure / connectivity
- 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!
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: further knowledge won’t help
  - Ideally simulation would incorporate this variability
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• Epistemic (e.g., bounded intervals or unknown distro parm)
  – Subjective, type-B, state of knowledge uncertainty
  – Reducible: more data or information, would make uncertainty estimation more precise
  – Fixed value in simulation, e.g., elastic modulus, but not well known
Uncertainty Quantification

- Identify and characterize uncertain variables (may not be normal, uniform)
- **Forward propagate**: quantify the effect that (potentially correlated) uncertain (nondeterministic) input variables have on model output:

\[ \text{Input Variables } u \] (physics parameters, geometry, initial and boundary conditions)
\[ \rightarrow \] Computational Model
\[ \rightarrow \] Variable Performance Measures \( f(u) \)

(possibly given distributions)

(here assumed a black-box)

Potential Goals:
- based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)
- **validation**: is the model sufficient for the intended application?
- quantification of margins and uncertainties (QMU): how close are uncertainty-aware code predictions to performance expectations or limits?
- quantify uncertainty when using calibrated model to predict
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
Black-box UQ Workhorse: Random 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**
  
  $$\bar{\bar{T}} = \frac{1}{N} \sum_{i=1}^{N} T(u^i)$$

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

- **full PDF(probabilities)**

- Monte Carlo sampling
- Quasi-Monte Carlo
- Centroidal Voronoi Tessalation (CVT)
- Latin hypercube (stratified) sampling: better convergence; stability across replicates

Robust, but slow convergence: $O(N^{-1/2})$, independent of dimension (in theory)
Challenges: Simulation-based UQ

• Similar to optimization for simulation-based engineering
• Need statistics of response function $f$, e.g., $\mu_f$, $\sigma_f$, $\text{Prob}[f > f_{\text{critical}}]$
• Characteristics/issues:
  • input parameters characterized by PDFs or intervals
  • no explicit function for $f(x_1, x_2)$
  • expensive to evaluate $f(x_1, x_2)$ (may fail; limited number of samples)
  • noisy, non-smooth, multi-modal
  • dimension of parameter space
  • complex, coupled systems
  • evaluate small probabilities

UQ in DAKOTA attempts to mitigate: a mix of statistics, nonlinear optimization, numerical integration, and surrogate modeling enables robust and efficient UQ methods.
Random Sampling for Coupled Systems

- Sampling: not the most efficient UQ method
- However, easy to implement and transparent to trace sample realizations through complex multi-code UQ studies

Input Distributions
N samples of X

Simulation Model 1

Simulation Model 2

Additional Inputs for Simulation 2

Output Distributions
N realizations of f(X)

Measure 1

Measure 2

Additional Inputs for Simulation 3

Simulation Model 3

Additional Inputs for Simulation 3

Input Distributions

Simulation Model 1

Simulation Model 2

Simulation Model 3
Challenge: Calculating Potentially Small Probability of Failure

- Given uncertainty in materials, geometry, and environment, how to determine likelihood of failure: $\text{Probability}(T \geq T_{\text{critical}})$?
- Perform 10,000 LHS samples and count how many exceed threshold; (better) perform adaptive importance sampling

**Mean value:** make a linearity (and possibly normality) assumption and project; great for many parameters with efficient derivatives!

$$\mu_T = T(\mu_u)$$

**Reliability:** directly determine input variables which give rise to failure behaviors by solving an optimization problem for a most probable point (MPP) of failure

$$\sigma_T = \sum_i \sum_j \text{Cov}_u(i, j) \frac{dg}{du_i} (\mu_u) \frac{dg}{du_j} (\mu_u)$$

minimize $u^T u$

subject to $T(u) = T_{\text{critical}}$

*All the usual nonlinear optimization tricks apply...*
Efficient Global Reliability Analysis: GP Surrogate + MMAIS (B.J. Bichon)

- 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; addresses nonlinear and multimodal challenges

Gaussian process model (level curves) of reliability limit state with

10 samples

failure region

safe region

28 samples

exploit

explore
Challenge: Dimension Selection and Resolution

• Open (impossible?) challenge: “needle in a haystack” UQ problems (local features without global trends, e.g., interatomic potential minimization or rare AND isolated event); perhaps a challenging exhaustive global optimization problem; not practical for expensive models

• Tractable challenge: identify and resolve uncertainties in crucial input dimensions, e.g., reduce from $O(1000)$ to $O(10)$ key parameters
  – advance screening (global sensitivity), then UQ
  – online, adaptive methods for stochastic expansions
  – leverage gradient information if available cheaply

• While similar for polynomial chaos and interpolation-based stochastic collocation (and they are essentially equivalent in practice), examples here are for PCE.
Generalized Polynomial Chaos Expansions (PCE)

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

\[ R = \sum_{j=0}^{P} \alpha_j \Psi_j(\xi) \]

\[ R(\xi) \approx f(u) \]

- Intrusive or non-intrusive
- Wiener-Askey Generalized PCE: optimal basis selection leads to exponential convergence of statistics

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Density function</th>
<th>Polynomial</th>
<th>Weight function</th>
<th>Support range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>( \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} )</td>
<td>Hermite ( H_n(x) )</td>
<td>( e^{-\frac{x^2}{2}} )</td>
<td>( [-\infty, \infty] )</td>
</tr>
<tr>
<td>Uniform</td>
<td>( \frac{1}{2} )</td>
<td>Legendre ( P_n(x) )</td>
<td>1</td>
<td>( [-1, 1] )</td>
</tr>
<tr>
<td>Beta</td>
<td>( \frac{(1-x)^\alpha(1+x)^\beta}{2^{\alpha+\beta}1B(\alpha+1,\beta+1)} )</td>
<td>Jacobi ( P_n^{(\alpha,\beta)}(x) )</td>
<td>( (1-x)^\alpha(1+x)^\beta )</td>
<td>( [-1, 1] )</td>
</tr>
<tr>
<td>Exponential</td>
<td>( e^{-x} )</td>
<td>Laguerre ( L_n(x) )</td>
<td>( e^{-x} )</td>
<td>( [0, \infty] )</td>
</tr>
<tr>
<td>Gamma</td>
<td>( \frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)} )</td>
<td>Generalized Laguerre ( L_n^{(\alpha)}(x) )</td>
<td>( x^\alpha e^{-x} )</td>
<td>( [0, \infty] )</td>
</tr>
</tbody>
</table>

- Can also numerically generate basis orthogonal to empirical data (PDF/histogram)
Forming PCE/SC Expansions
(for PCE, using $R_i$ to estimate $\alpha_j$)

Random sampling: PCE

*Expectation (sampling)*:
- Sample w/i distribution of $x$
- Compute expected value of product of $R$ and each $Y_j$

*Linear regression ("point collocation")*:

\[ \Psi \alpha = R \]

Tensor-product quadrature: PCE/SC

Tensor product of 1-D integration rules, e.g., Gaussian quadrature

Smolyak Sparse Grid: PCE/SC

Cubature: PCE

Stroud and extensions (Xiu, Cools): optimal multidimensional integration rules
Adaptive Approaches: Emphasize Key Dimensions

- Uniform p-refinement
  - Stabilize 2-norm of covariance
- Adaptive p-refinement
  - Estimate main effects/VBD to guide
- h-adaptive: identify important regions and address discontinuities
- h/p-adaptive: p for performance; h for robustness
Comparison of PCE/SC Approaches

![Comparison of PCE/SC Approaches](image)
Extend Scalability through Derivative Enhancement

- Leverage more data at each model evaluation (typically N+1 for gradients)
- PCE: linear regression with derivatives (simply additional equations)
- SC: gradient-enhanced interpolants (more challenging) via cubic Lagrange splines or Hermite polynomials
- EGRA: gradient-enhanced Kriging/co-Kriging. Interpolates function values and gradients
Interval Estimation Approach (Probability Bounds Analysis)

- **Propagate intervals through simulation code**
- **Outer loop:** determine interval on statistics, e.g., mean, 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 sampling, PCE, etc., to determine the CDFs or moments with respect to the aleatory variables

\[
\begin{align*}
\min_{u_E} f_{STAT}(u_A \mid u_E) \\
\quad \quad u_{LB} \leq u_E \leq u_{UB} \\
\quad \quad u_A \sim F(u_A ; u_E)
\end{align*}
\]

\[
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\end{align*}
\]
Interval Analysis can be Tractable for Large-Scale Apps

Converge to more conservative bounds with 10—100x less evaluations
UQ Not Addressed Here

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

• Production Bayesian analysis capability
• Bayesian approaches: Bayesian belief networks, Bayesian updating, Robust Bayes, etc.
• Scenario evaluation
• UQ algorithm efficiency is crucial when combining algorithms, e.g., for optimization under uncertainty, robust optimization, or nested uncertainty analysis

• Some progress: address high dimensionality with adaptive methods and derivative-enhancement

• Address expense and nonlinearity in part through global surrogate models

• To conclude: a few examples of
  – coupling
  – complex systems
UQ for Coupled Multi-Physics

- Can we efficiently propagate UQ across scales/disciplines?
- Naively wrapping multi-physics with UQ often too costly
- Can we invert loops and perform multi-physics analysis on UQ-enriched simulations (couple based on scalar statistics, random fields, stochastic processes)?

Source: CASL (DOE Energy Innovation Hub)
Multi-Physics, Multi-Fidelity, Heterogeneous UQ

- Component-level uncertainty propagation via stochastic expansions
- Stochastic dimension reduction at component interfaces
- Strongly coupled solver technology for coupled stochastic problems
- Stochastic upscaling for low-fidelity models
- Stochastic sensitivities with respect to system components

Component 1
\[ v_2 = G_1(v_1, p_1) = g_1(u_1(v_1), p_1) \text{ s.t. } f_1(u_1, v_1, p_1) = 0 \]

Component 2
\[ v_2 = G_2(v_2, p_2) = g_2(u_2(v_2), p_2) \text{ s.t. } f_2(u_2, v_2, p_2) = 0 \]

Equations
\[
\begin{align*}
  v_2 - G_1(v_1, p_1) &= 0 \\
  v_1 - G_2(v_2, p_2) &= 0
\end{align*}
\]

Newton Step
\[
\begin{align*}
  \Delta v_1 &= \left[ \frac{dG_1}{dv_1} \right]^{-1} \left[ \frac{dG_1}{dp_1} \right] \Delta p_1 - G_1(v_1, p_1) \\
  \Delta v_2 &= \left[ \frac{dG_2}{dv_2} \right]^{-1} \left[ \frac{dG_2}{dp_2} \right] \Delta p_2 - G_2(v_2, p_2)
\end{align*}
\]

High-fidelity Multi-physics Component Model (Core)

Low-fidelity Network Plant Model

Graphics courtesy: Rod Schmidt, BRSC project
Electrical Modeling Complexity

ASIC: 1000s to millions of devices

Large Digital Circuit (e.g., ASIC)

Sub-circuit (analog)

Single Device

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

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

(G. Gray, M. M-C, SNL)
Hierarchical/Network Structure

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

- Atmospheric entry vehicles are subject to turbulent flow, complex chemical reactions, thermal and pressure loads.
- Example goal: assess uncertainty in loads imposed on structures without running costly CFD over many scenarios (typically can’t afford full coupling).
- Need: random field characterization of uncertainty from CFD and efficient way to assess effect on structural dynamics.

NASA (public domain)
FSI: Nuclear Reactor
Grid-to-rod Fretting Failure

• Clad failure can result from rod-spring interactions
  – Induced by flow vibration
  – Amplified by irradiation-induced grid spacer growth and spring relaxation

• Power uprates and burnup increase potential for fretting failures (leading cause of fuel failures in PWRs)

• Ideally: High-fidelity, fluid structural interaction tool to predict uncertainty in gap, turbulent flow excitation, rod vibration and wear

Sources: CASL DOE
Energy Innovation Hub,
Roger Lu, Westinghouse

Spacer grid cell

1 Fuel

2 Fuel

3 Fuel
Possible Research Directions

GOAL: Advanced efficient, robust, accurate UQ methods for validation, extrapolation, and risk-informed decisions with expensive computational models

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

To contribute, understand: (1) an applied math or computational engineering / science discipline, (2) statistics / probability, and (3) computation

Thank you for your attention!
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