Uncertainty Quantification Algorithms and Software Enabling V&V

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Optimization and Uncertainty Quantification

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Advanced algorithms enable robust, efficient uncertainty quantification for validating models with experimental data and making credible predictions.

- Uncertainty quantification for credible simulation
- UQ algorithms research in DAKOTA
  - Aleatory UQ methods: beyond Monte Carlo
  - Challenges in epistemic UQ methods
- Sandia’s QASPR program: computational model-based system qualification

Slide credits: Mike Eldred, Laura Swiler, Barron Bichon, Joe Castro, Genetha Gray, Bill Oberkampf, Matt Kerschen, others
Insight from Computational Simulation

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

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

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

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

Hurricane Katrina: weather, logistics, economics, human behavior
Ultimate purpose (arguably): insight, prediction, and risk-informed decision-making → need credibility for intended application
Uncertainties to Quantify

A partial list of uncertainties affecting computational model results

• typical parametric uncertainty, incl. random fields/processes
  – physics/science parameters
    (e.g., cross sections, reaction rates; seismic spectra)
  – statistical variation, inherent randomness
  – operating environment, interference
    (e.g., debris, corrosion, oxidation, and erosion)
  – initial, boundary conditions; forcing
  – geometry / structure / connectivity (e.g., fuel rod packing)
  – material properties
  – manufacturing quality

• model form / accuracy (e.g., equation of state)

• program: requirements, technical readiness levels
  (also economics, regulations, schedules)

• human reliability, subjective judgment, linguistic imprecision

• numerical accuracy: mesh, solver, approximation error

• experimental error: measurement error, bias
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?
- validation with experimental data ensembles

Need to make risk-informed decisions, based on an assessment of uncertainty
Categories of Uncertainty

Often useful algorithmic distinctions, but not always a clear division

• **Aleatory** *(think probability density function)*
  – Inherent variability (e.g., in a population)
  – Irreducible uncertainty – can’t reduce it by further knowledge

• **Epistemic** *(think bounded intervals)*
  – Subjective uncertainty
  – Related to what we don’t know
  – Reducible: If you had more data or more information, you could make your uncertainty estimation more precise

• In practice, people try to transform or translate uncertainties to the aleatory type and perform sampling and/or parametric analysis
Uncertainty Quantification

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

Potential Goals:

- based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)
- 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
Uncertainty Quantification Example

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

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

- Probability distribution of temperatures
- Correlations (trends) and sensitivity of temperature
- Mean($T$), StdDev($T$), Probability($T \geq T_{\text{critical}}$)
Given distributions of $u_1, \ldots, u_N$, UQ methods...

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

...calculate statistical info on outputs $T(u_1, \ldots, u_N)$
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)
Calculating Probability of Failure

• Given uncertainty in materials, geometry, and environment, determine likelihood of failure
  \[ \text{Probability}(T \geq T_{\text{critical}}) \]

• Could perform 10,000 Monte Carlo samples and count how many exceed the threshold...

• Or directly determine input variables which give rise to failure behaviors by solving an optimization problem.

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

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

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

DAKOTA optimization, sensitivity analysis, parameter estimation, uncertainty quantification

parameters (design, UC, state)

Computational Model (simulation)

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

response metrics

Nominal Optimized
DAKOTA C++/OO Framework Goals

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

![Algorithm Hierarchy Diagram]

-algorithms hierarchy-
Flexibility with Models & Strategies

**DAKOTA models** map inputs to response metrics of interest:

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

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

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

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

**DAKOTA strategies** enable flexible combination of multiple models and algorithms.

- nested
- layered
- cascaded
- concurrent
- adaptive / interactive
Alternatives to Sampling

LHS sampling is robust, trusted, ubiquitous, but advanced methods may offer advantages:

• for a modest number of random variables, polynomial chaos expansions may converge considerably faster to statistics of interest

• if principal concern is with failure modes (tail probabilities), consider global reliability methods
Approximate response stochasticity 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
- Nonintrusive: estimate response coefficients using sampling (expectation), quadrature/cubature (num integration), point collocation (regression)

Wiener-Askey Generalized PCE with adaptivity
- Tailor basis: optimal basis selection leads to exponential convergence rates

<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+1}B(\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{1}{\Gamma(\alpha+1)} x^\alpha e^{-x} )</td>
<td>Generalized Laguerre ( L_n^{(\alpha)}(x) )</td>
<td>( x^\alpha e^{-x} )</td>
<td>([0, \infty])</td>
</tr>
</tbody>
</table>

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

Residual in PCE CDF for Lognormal Ratio, increasing simulations

Hermite basis, lognormal distributions
- quad order = exp order + 1, $10^4$ samples on PCE
- quad order = exp order + 1, $10^5$ samples on PCE
- quad order = exp order + 1, $10^6$ samples on PCE
- pt colloc ratio = 2, $10^4$ samples on PCE
- pt colloc ratio = 2, $10^5$ samples on PCE
- pt colloc ratio = 2, $10^6$ samples on PCE
- exp samples, exp order = 10, $10^4$ samples on PCE
- exp samples, exp order = 10, $10^5$ samples on PCE
- exp samples, exp order = 10, $10^6$ samples on PCE

CDF for Rosenbrock Problem, expansion order = 4, varying distribution/basis

CDF

- Normal: Hermite chaos
- Normal: $10^4$ LHS
- Uniform: Legendre chaos
- Uniform: $10^4$ LHS
- Exponential: Laguerre chaos
- Exponential: $10^4$ LHS
- Beta: Jacobi chaos
- Beta: $10^4$ LHS
- Gamma: gen Laguerre chaos
- Gamma: $10^4$ LHS
- mixed: Askey chaos
- mixed: $10^4$ LHS
**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)**

\[
\begin{align*}
\text{minimize} & \quad u^T u \\
\text{subject to} & \quad G(u) = \bar{z}
\end{align*}
\]

Region of \( u \) values where \( T \geq T_{\text{critical}} \) map \( T_{\text{critical}} \) to a probability.
Reliability: Algorithmic Variations

Many variations possible to improve efficiency, including in DAKOTA…

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

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

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

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

  - 1st-order: \[ p(g \leq z) = \Phi(-\beta_{cdf}) \]
  - 2nd-order: \[ p = \Phi(-\beta) \prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta \kappa_i}} \]

  curvature correction

- **MPP search algorithm**: Sequential Quadratic Prog. (SQP) vs. Nonlinear Interior Point (NIP)

- **Warm starting (for linearizations, initial iterate for MPP searches)**: speeds convergence when increments made in: approximation, statistics requested, design variables
**Efficient Global Reliability Analysis**

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

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

![Graph showing GP surrogate and True fn from Jones, Schonlau, Welch, 1998](image)
Efficient Global Reliability Analysis

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*Gaussian process model of reliability limit state with 10 samples* vs *28 samples*
• Epistemic uncertainty: insufficient information to specify a probability distribution
• Subjective, reducible, or lack-of-knowledge uncertainty (given more resources to gather information, could reduce the uncertainty)
• For example:
  – “I expect this parameter to have a lognormal distribution, but only know bounds on its mean and standard deviation,” or
  – Dempster-Shafer belief structures: “basic probability assignment” for each interval where the uncertain variable may exist; contiguous, overlapping, or gapped
Second-order probability
- Two levels: distributions/intervals on distribution parameters
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distributions)
- Strong regulatory history (NRC, WIPP).

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

<table>
<thead>
<tr>
<th>Source</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>10% 90%</td>
</tr>
<tr>
<td>Source 2</td>
<td>10% 70% 20%</td>
</tr>
<tr>
<td>Source 3</td>
<td>33% 33% 33%</td>
</tr>
</tbody>
</table>
# DAKOTA UQ Algorithms Summary

**Goal:** bridge robustness/efficiency gap

<table>
<thead>
<tr>
<th></th>
<th>Production</th>
<th>New</th>
<th>Under dev.</th>
<th>Planned</th>
<th>Collabs.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sampling</strong></td>
<td>LHS/MC, QMC/CVT</td>
<td>IS/AIS/MMAIS, Incremental LHS</td>
<td></td>
<td>Bootstrap, Jackknife</td>
<td>Gunzburger</td>
</tr>
<tr>
<td><strong>Reliability</strong></td>
<td>1st/2nd-order local: MVFOSM/SOSM, x/u AMV/AMV²/ AMV+/AMV²+, x/u TANA, FORM/SORM</td>
<td>Global: EGRA</td>
<td></td>
<td></td>
<td>Renaud, Mahadevan</td>
</tr>
<tr>
<td><strong>Polynomial chaos/ Stochastic collocation</strong></td>
<td></td>
<td>Wiener-Askey gPC: sampling, quad/cubature, pt collocation SC: quadrature</td>
<td>SC: cubature gPC/SC: arbitrary input PDFs</td>
<td>Adaptivity, Wiener-Haar</td>
<td>Ghanem</td>
</tr>
<tr>
<td><strong>Other probabilistic</strong></td>
<td></td>
<td></td>
<td></td>
<td>Dimension reduction</td>
<td>Youn</td>
</tr>
<tr>
<td><strong>Epistemic</strong></td>
<td>Second-order probability</td>
<td>Dempster-Shafer evidence theory</td>
<td></td>
<td>Bayesian, Imprecise probability</td>
<td>Higdon, Williams, Ferson</td>
</tr>
<tr>
<td><strong>Metrics</strong></td>
<td>Importance factors, Partial correlations</td>
<td>Main effects, Variance-based decomposition</td>
<td></td>
<td>Stepwise regression</td>
<td>Storlie</td>
</tr>
</tbody>
</table>
Neutron Radiation Exposure
Degrades Electronics

- Military requirement: certify to hostile environment

neutrons create damage

Emitter (n-type)
Base (p-type)
Collector (n-type)
damage degrades gain

Prerad:
$\beta_0 = 150$

Gain ($\Omega$)

Seconds after peak neutron pulse
*Military requirement: certify to hostile environment*

*SPR dismantled end of FY06 to improve security posture*
Neutron Radiation Exposure
Degrades Electronics

QASPR (Qualification Alternatives to Sandia Pulse Reactor)
methodology will certify qualification via modeling &
simulation with quantified uncertainty

- Military requirement: certify to hostile environment
- SPR dismantled end of FY06 to improve security posture

neutrons create damage

Emmitter (n-type)
Base (p-type)
Collector (n-type)
damage degrades gain

QASPR
QUALIFICATION ALTERNATIVES TO SPR
quantified uncertainty

Prerad:
\( \beta_0 = 150 \)
QASPR: Science-Based Engineering Methodology For Qualification

Risk Informed Decisions

Qualification Evidence

select experiments in alternate facilities

UQ

EC

M&S

uncertainty quantification

validation

high performance, multi-fidelity, predictive computational modeling

γ,n – 100 ms long pulse

ion – 100 μs short pulse

γ,n – 100 ms

ion – 100 μs
V&V for QASPR Components

Developing formal V&V plans
Each computational code subject to code and solution verification
UQ used to validate device model response against data ensembles
Ultimately systems (circuit) V&V for qualification
Device Prototype: UQ Extrapolation to SPR

- Calibrated to other facilities, CHARON fills SPR gap
  - Uncertainty & bias characterized by 2 degrees of freedom
    - facility multiplier
    - device multiplier

- Uncertainty quantified with D.O.E + statistical approach

End UQ Methodology Goal: Best Estimate + Uncertainty Prediction for SPR
Model Validation: Blind Prediction

- Fairchild response data within SPR hidden

- First prototype of the QASPR methodology (and real validation of the QASPR system)

- Prediction + Uncertainty (+/-2σ device and facility uncertainty)

Transient Device Damage Response
All Experiments (grey), Mean (black), +/-2 Sigma (blue)

UQ algorithms have a critical role in system validation
• Fairchild response data within SPR hidden

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**Transient Device Damage Response**

SPR 13268q1 (black) and Simulation bounds (yellow)

+/- 1-2% vertical error on experimental measurement

**UQ algorithms have a critical role in system validation**
Model Validation: Blind Prediction

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Transient Device Damage Response
SPR 13564q1 (black) and Simulation bounds (yellow)

+/− 1-2% vertical error on experimental measurement

UQ algorithms have a critical role in system validation
Electrical Modeling Complexity

**complex device models + replicates in circuits**

- **ASIC:** 1000s to millions of devices
- **Large Digital Circuit** (e.g., ASIC)
- **Sub-circuit** (analog)
- **Single Device**

**device: 1 to 100s of params**

- **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)

Simulation time grows exponentially (G. Gray, M. M-C)
UQ: Mitigate Explosion of Factors!

- Consider bounding parameter sets?
- Exploit natural hierarchy or network structure?
- Use surrogate/macro-models as glue between levels?
- *Need approaches curbing the curse of dimensionality*
Summary

Advanced algorithms enable robust, efficient uncertainty quantification for validating models with experimental data and making credible predictions.

• Credible simulations must deliver best estimate + uncertainty.
• Uncertainty quantification algorithms are essential in validation and calibration under uncertainty
• Complex/large-scale/multi-scale/multi-physics simulations demand research in advanced efficient UQ methods

Thank you for your attention!

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http://www.cs.sandia.gov/DAKOTA
Abstract

Uncertainty Quantification Algorithms and Software Enabling V&V

Computational simulations are increasingly used for risk-informed decision making in the presence of uncertainties. To be credible, they must deliver not only a best estimate of performance, but also its degree of variability or uncertainty. Uncertainty quantification (UQ) algorithms compute the effect of uncertain input variables on simulation response metrics of interest, enabling model validation and subsequent credible risk assessment.

I will survey UQ algorithms research addressing both aleatory (inherent) and epistemic (lack-of-knowledge) uncertainties. For example, advanced reliability analysis and polynomial chaos expansion methods available in Sandia's DAKOTA toolkit offer substantial efficiency advantages over ubiquitous Monte Carlo sampling. Application to electrical circuit calibration and validation in the QASPR (Qualification Alternatives to Sandia's Pulsed Reactor) program will demonstrate UQ algorithms in an extrapolation context and motivate the need to develop hierarchical UQ techniques for systems analysis.