From Uncertainty to Credibility: UQ Algorithms and Research Challenges

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Optimization and Uncertainty Quantification

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2008 CSRI Summer Lecture Series
Sandia National Laboratories
Albuquerque, NM
Ph.D., Computational and Applied Mathematics, NC State
- mathematics, statistics, computer science, immunology
- nondeterministic model calibration (HIV)
- internship at Fred Hutchinson Cancer Research Center

SNL since 2005 to fulfill goals:
- optimization focus (surprise: uncertainty quantification)
- develop algorithms; production software implementation in DAKOTA
- work with science/engineering application customers;
  let their unmet needs drive research and software
To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.

- Ubiquitous computational simulation
- Why consider uncertainty quantification (UQ)
- Propagating uncertainty through models
  - Intro to UQ methods
  - Advanced UQ methods in DAKOTA
- Reliability-based MEMS design (OPT+UQ)
- Research challenges in electrical circuit UQ

*Slide credits: Mike Eldred, Laura Swiler, Barron Bichon, Genetha Gray, Bill Oberkampf, Matt Kerschen, others*
Sandia’s Mission Focus Relies on Strong Science and Engineering

Computational and Information sciences

Engineering Sciences

Materials Science and Technology

Microelectronics and Photonics

Pulsed Power

Bioscience

Sandia National Laboratories
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

Hurricane Katrina: weather, logistics, economics, human behavior

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

- Ultimate purpose of modeling and simulation is (arguably) insight, prediction, and decision-making → need credibility for intended application

- Historically: primary focus on modeling fidelity

**Graphic credit: Bill Oberkampf**
Credible Simulation: Beyond Nominal

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

Slide credit: Bill Oberkampf
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.

Related 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?
Algorithms for Computational Modeling & Simulation

Are you sure you don’t need verification?!

- System Design
- Geometric Modeling
- Meshing
- Physics
- Model Equations
- Discretization
- Partitioning and Mapping
- Optimization and UQ
- Adapt
- Time integration
- Nonlinear solve
- Linear solve
- Information Analysis & Validation

Improved design and understanding
• A single optimal design or nominal performance prediction is often insufficient for
  – decision making / trade-off assessment
  – validation with experimental data ensembles

• Need to make risk-informed decisions, based on an assessment of uncertainty
Uncertainties to Quantify

A partial list of uncertainties affecting computational model 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
Categories of Uncertainty

(Often useful distinctions, but not always a clear line between them)

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

- **Epistemic** *(not in this talk, though a crucial research area)*
  - 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
To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.

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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
- $\text{Mean}(T)$, $\text{StdDev}(T)$, $\text{Probability}(T \geq T_{\text{critical}})$
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

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

Computational Model

Variable Performance Measures $f(u)$

Output Distributions

Typical method: Monte Carlo Sampling
Challenges to This Process

- Engineering application: propagate variability through a computer model.
- Need statistics of response function “f”, e.g., $\mu_f$, $\sigma_f$, Prob[$f > f_{\text{critical}}$].
- Characteristics of response function:
  - 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

Research Question:
Which is more accurate?
- compute statistics from the $f(x_1, x_2)$ sample values, or
- construct an approximation model based on the $f(x_1, x_2)$ values and then compute statistics from the model?
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

Computational Model (simulation)

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

Nominal vs. 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)*

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**DAKOTA C++/OO Framework**

- **LHS/MC**
- **Iterator**
- **ParamStudy**
  - Vector
  - Center
  - MultiD
  - List
- **DoE**
  - DDACE
  - QMC/CVT
  - CCD/BB
  - PSUADE
- **Optimizer**
  - LeastSq
  - NLSSOL
  - NL2SOL
  - GN
- **UQ**
  - LHS/MC
  - DSTE
  - Reliability
  - SFEM/PCE
  - EGRA

**algorithms hierarchy**

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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**

**Strategy**

- **Optimization**
  - Hybrid
  - Surrogate Based
  - Pareto/Multi-Start

- **Uncertainty**
  - OptUnderUnc
  - UncOfOptima
  - 2nd Order Probability

- **Branch&Bound/PICO**
Sensitivity analysis techniques help determine which input variables are most important (perhaps for which to refine uncertainty estimates)

• Parameter Studies
  – Alter variables one at a time or on grid
  – Impractical in high dimension $d \sim$ (partitions

• Design of Computer Experiments (DACE) vs. Design of Experiments (DOE)
  – Box-Behnken
  – Central Composite
  – Factorial and fractional designs
  – Orthogonal Arrays

• Correlation Analysis
  – Linear correlation
  – Variance-based decomposition

• Morris One at a Time Sampling
SA: Orthogonal Arrays

- For each level of one factor, all levels of other factors occur equal number of times.
- **Orthogonality**: statistical independence between columns of the experimental design matrix (confounding factors cancel)
- Good for main effects, terrible for variable interactions
- Large OA databases available

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<tr>
<th>Exp. No</th>
<th>Var. 1</th>
<th>Var. 2</th>
<th>Var. 3</th>
<th>Var. 4</th>
<th>Var. 5</th>
<th>Var. 6</th>
<th>Var. 7</th>
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<td>1</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

Main effects of 7 variables, each with 2 levels, in 8 samples!
Given distributions of $u_1, \ldots, u_N$, UQ methods...

\[ T(u_1, \ldots, u_N) \]

\[ % \text{ in Bin} \]

Final Temperature Values
Quasi-Monte Carlo Sequences

- Deterministic sequences from a series of prime bases
- Designed to produce uniform random numbers on the interval [0,1]
- Low discrepancy
- Example: Halton sequences

<table>
<thead>
<tr>
<th>Sample Number</th>
<th>Base 2</th>
<th>Base 3</th>
<th>Base 5</th>
<th>Base 7</th>
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</thead>
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<tr>
<td>1</td>
<td>0.5000</td>
<td>0.3333</td>
<td>0.2000</td>
<td>0.1429</td>
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<td>2</td>
<td>0.2500</td>
<td>0.6667</td>
<td>0.4000</td>
<td>0.2857</td>
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<td>3</td>
<td>0.7500</td>
<td>0.1111</td>
<td>0.6000</td>
<td>0.4286</td>
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<td>4</td>
<td>0.1250</td>
<td>0.4444</td>
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<td>0.5714</td>
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<td>5</td>
<td>0.6250</td>
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<td>0.0400</td>
<td>0.7143</td>
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<td>0.3750</td>
<td>0.2222</td>
<td>0.2400</td>
<td>0.8571</td>
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<td>7</td>
<td>0.8750</td>
<td>0.5556</td>
<td>0.4400</td>
<td>0.0204</td>
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<td>8</td>
<td>0.0625</td>
<td>0.8889</td>
<td>0.6400</td>
<td>0.1633</td>
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<td>9</td>
<td>0.5625</td>
<td>0.0370</td>
<td>0.8400</td>
<td>0.3061</td>
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<tr>
<td>10</td>
<td>0.3125</td>
<td>0.3704</td>
<td>0.0800</td>
<td>0.4490</td>
</tr>
</tbody>
</table>

Halton sequences

Base 2 and Base 3

- Halton 100 points
- Halton 25 points
- Halton 10 points
Centroidal Voronoi Tessellation (CVT)

- Generates nearly uniform spacing over arbitrarily shaped parameter spaces (can also be used for non-uniform distributions)
- Origin: unstructured meshing for irregular domains
- Ideal for high dimensional volumetric sampling

Gunzburger, et al.: comparison of random sampling and CVT
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)
Generalized Polynomial Chaos Expansions

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{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>

- 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

CDF for Rosenbrock Problem, expansion order = 4, varying distribution/basis
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
Calculating Probability of Failure

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

**Final Temperature Values**

- 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.
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

Response Value
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

  - 1\(^{st}\)-order: \[
  \begin{align*}
  p(g \leq z) &= \Phi(-\beta_{cdf}) \\
  p(g > z) &= \Phi(-\beta_{ccdf})
  \end{align*}
  \]

  - 2\(^{nd}\)-order: \[
  p = \Phi(-\beta) \prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta \kappa_i}} \text{ curvature correction}
  \]

- **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 True fn and GP surrogate](image_url)

From Jones, Schonlau, Welch, 1998
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.

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Gaussian process model of reliability limit state with 10 samples

[Graph showing 10 sample points and two curves, labeled 'explore' and 'exploit']

Gaussian process model of reliability limit state with 28 samples

[Graph showing 28 sample points and two curves, labeled 'explore' and 'exploit']
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Shape Optimization of Compliant MEMS

- Micro-electromechanical system (MEMS): typically made from silicon, polymers, or metals; used as micro-scale sensors, actuators, switches, and machines
- MEMS designs are subject to substantial variability and lack historical knowledge base. Materials and micromachining, photo lithography, etching processes all yield uncertainty.
- Resulting part yields can be low or have poor cycle durability
- Goal: shape optimize finite element model of bistable switch to...
  - Achieve prescribed reliability in actuation force
  - Minimize sensitivity to uncertainties (robustness)

<table>
<thead>
<tr>
<th>variable</th>
<th>mean</th>
<th>std. dev.</th>
<th>distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta w$</td>
<td>-0.2 $\mu m$</td>
<td>0.08</td>
<td>normal</td>
</tr>
<tr>
<td>$S_r$</td>
<td>-11 Mpa</td>
<td>4.13</td>
<td>normal</td>
</tr>
</tbody>
</table>
Tapered Beam Bistable Switch: Performance Metrics

13 design vars $d$: $W_i, L_i, \theta_i$

Key relationship: force vs. displacement

Typical design specifications:
- actuation force $F_{\text{min}}$ reliably 5 $\mu$N
- bistable ($F_{\text{max}} > 0$, $F_{\text{min}} < 0$)
- maximum force: $50 < F_{\text{max}} < 150$
- equilibrium $E_2 < 8$ $\mu$m
- maximum stress < 1200 MPa
Optimization Under Uncertainty

Rather than design and then post-process to evaluate uncertainty… actively design optimize while accounting for uncertainty/reliability metrics $s_u(d)$, e.g., mean, variance, reliability, probability:

\[
\begin{align*}
\text{min} \quad & f(d) + W s_u(d) \\
\text{s.t.} \quad & g_l \leq g(d) \leq g_u \\
& h(d) = h_t \\
& d_l \leq d \leq d_u \\
& a_l \leq A_i s_u(d) \leq a_u \\
& A e s_u(d) = a_t
\end{align*}
\]

(nested paradigm)

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

simultaneously reliable and robust designs

\[
\begin{align*}
\text{max} \quad & \mathbb{E} [F_{\text{min}}(d, x)] \\
\text{s.t.} \quad & 2 \leq \beta_{ccdf}(d) \\
& 50 \leq \mathbb{E} [F_{\text{max}}(d, x)] \leq 150 \\
& \mathbb{E} [E_2(d, x)] \leq 8 \\
& \mathbb{E} [S_{\text{max}}(d, x)] \leq 3000
\end{align*}
\]

13 design vars $d$: $W_p, L_p, q_i$
2 random variables $x$: $\Delta W, S_r$

displacement

force

switch contact
RBDO Finds Optimal & Robust Design

Close-coupled results: DIRECT / CONMIN + reliability method yield **optimal** and **reliable/robust** design:

<table>
<thead>
<tr>
<th>l.b.</th>
<th>metric</th>
<th>u.b.</th>
<th>initial $d^0$</th>
<th>MVFOSM</th>
<th>AMV$^2+$</th>
<th>FORM</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$E[F_{\text{min}}]$ (μN)</td>
<td>5.376</td>
<td>-5.896</td>
<td>-6.188</td>
<td>-6.292</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>$E[F_{\text{max}}]$ (μN)</td>
<td>68.69</td>
<td>50.01</td>
<td>57.67</td>
<td>57.33</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E[E_2]$ (μm)</td>
<td>8</td>
<td>4.010</td>
<td>5.804</td>
<td>5.990</td>
<td>6.008</td>
</tr>
<tr>
<td></td>
<td>$E[S_{\text{max}}]$ (MPa)</td>
<td>1200</td>
<td>470</td>
<td>1563</td>
<td>1333</td>
<td>1329</td>
</tr>
<tr>
<td></td>
<td>AMV$^2+$ verified $\beta$</td>
<td>3.771</td>
<td>1.804</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FORM verified $\beta$</td>
<td>3.771</td>
<td>1.707</td>
<td>1.784</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>
# DAKOTA UQ Algorithms Summary

**Goal:** bridge robustness/efficiency gap

<table>
<thead>
<tr>
<th>Methodology</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>1\textsuperscript{st}/2\textsuperscript{nd}-order local: MVFOSM/SOSM, x/u AMV/AMV\textsuperscript{2}/AMV+ AMV\textsuperscript{2+}, 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>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></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>Stepwise regression</td>
<td></td>
<td>Storlie</td>
</tr>
</tbody>
</table>
To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.

- Ubiquitous computational simulation
- Why consider uncertainty quantification (UQ)
- Propagating uncertainty through models
  - Intro to UQ methods
  - Advanced UQ methods in DAKOTA
- Reliability-based MEMS design (OPT+UQ)
- Research challenges in electrical circuit UQ
Electrical Modeling Complexity

- **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)

ASIC: 1000s to millions of devices

Large Digital Circuit (e.g., ASIC)

Sub-circuit (analog)

Single Device

Circuit Board

Sub-circuit: 10s to 100s of devices

Device: 1 to 100s of params

Simulation time grows exponentially (G. Gray, M. M-C)
• Circuit analysis challenges
  – network of nonlinearly coupled components, feedback loops, staged behavior, or discrete digital logic, mandating all-at-once circuit solution techniques
  – long simulation time involving iterative solvers (often hours to simulate microseconds, particularly in oscillating electronics);
  – combination of analog and digital circuits: consider separately or together
    • analog circuits typically < 100 devices, including replicates, less predictable topology across designs
    • digital circuits 1,000 to 1,000,000 transistors (identical or similar), small number of well-defined connection types.

• Typical parametric uncertainties:
  – process parameters (e.g., diffusion times, oven temperatures)
  – physical parameters (e.g., line widths, channel doping)
  – model parameters (e.g., BSIM3 transistor compact model)
  – electrical parameters (e.g., line resistance, saturation current, threshold voltage)

• Mapping reality to compact model parameters not always easy; compact model may be more behavioral than physics-based
UQ: Explosion of Factors!

complex device models + replicates in circuits

• Tor Fjeldy radiation photocurrent models for transistors
  – 20 model parameters, three levels for each (low, nominal, high) ~ 3 billion combinations
  – not practical via factorial brute force, but LHS might miss extreme “corner” behaviors
  – 6 devices in circuit of interest; mitigated via OAs

• Simple voltage regulator circuit
  – 4 BJTs, 1 MOSFET, 17 resistors, 1 capacitor, 1 zener diode
  – over 100 parameters if considered naively
  – mitigate by determining parameter sets giving rise to low, nominal, high response for each device

• CMOS 7 ViArray: generic ASIC implementation platform
  – Approx 1 million transistors
  – adding parasitics yields a simulation with millions of resistors, capacitors, inductors
  – mitigated by grouping within process layers

Approaches curbing the curse of dimensionality crucial in analyzing these kinds of systems!
Zener Low-Nominal-High Models

• For single device, perform LHS samples of 20 parameters

• Determine 3 sets of parameters giving rise to nominal and extreme device response

• When performing circuit UQ, sample uniformly from L,N,H and set all 20 parameters accordingly in the full simulation
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?
Other Relevant Technologies

- Apply existing reliability and polynomial chaos methods; benefit of embedded techniques?

- Principal components analysis (PCA, SVD, POD), reduced-order modeling techniques: only vary uncorrelated parameters

- Surrogate/macro modeling, insert current/voltage sources representative of the effect of uncertainty

- Leverage structure of network, DAE system under the hood; automatic structure analysis, macro-model creation?
To be credible, simulations must deliver not only a best estimate of performance, but also its degree of variability or uncertainty.

- Uncertainty quantification algorithms are essential in credible simulation

- Complex, large-scale simulations demand research in advanced efficient UQ methods

Thank you for your attention!

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http://www.sandia.gov/~briadam
Abstract

- 2008 CSRI Summer Lecture Series
- Title: "From uncertainty to credibility: UQ algorithms and research challenges"
- Speaker: Brian Adams (Org. 1411)
- Date/Time: Wednesday, July 2, 3-4pm (MST)
- Location:
  - NM: CSRI/90
  - CA: 915/S145

Abstract:

Computational simulations are routinely used to assess the performance, reliability, and safety of existing and proposed systems, and are increasingly used for risk-informed decision making in the presence of uncertainties. To be credible, simulations 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 response metrics of interest, enabling risk assessment, model calibration, and model validation. In this talk, I will motivate simulation-based UQ with examples from electrical circuit and MEMS design. I will survey methods from ubiquitous Monte Carlo sampling through more advanced reliability analysis and polynomial chaos expansions available in Sandia's DAKOTA toolkit. In particular, DAKOTA's reliability analysis methods employ a mix of probability, optimization, and surrogate (meta-) modeling to efficiently perform UQ.

Challenges in large-scale electrical circuit UQ will motivate unmet algorithm research needs.
Epistemic UQ

Second-order probability
- Two levels: distributions/intervals on distribution parameters
  - Outer level can be epistemic (e.g., interval)
  - Inner level can be aleatory (probability distrs)
  - 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

New

New
Epistemic Uncertainty Quantification

- Epistemic uncertainty refers to the situation where one does not know enough to specify a probability distribution on a variable.
- Sometimes it is referred to as subjective, reducible, or lack of knowledge uncertainty.
- The implication is that if you had more time and resources to gather more information, you could reduce the uncertainty.
- Initial implementation in DAKOTA uses Dempster-Shafer belief structures. For each uncertain input variable, one specifies “basic probability assignment” for each potential interval where this variable may exist.
- Intervals may be contiguous, overlapping, or have “gaps”.

<table>
<thead>
<tr>
<th>Variable 1</th>
<th>Variable 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPA=0.5</td>
<td>BPA=0.5</td>
</tr>
<tr>
<td>BPA=0.3</td>
<td>BPA=0.3</td>
</tr>
<tr>
<td>BPA=0.2</td>
<td>BPA=0.2</td>
</tr>
</tbody>
</table>
- Look at various combinations of intervals. In each joint interval “box”, one needs to find the maximum and minimum value in that box (by sampling or optimization).
- Belief is a lower bound on the probability that is consistent with the evidence.
- Plausibility is the upper bound on the probability that is consistent with the evidence.
- Order these beliefs and plausibility to get CDFs.
- Draws on the strengths of DAKOTA
  - Requires surrogates
  - Requires sampling and/or optimization for calculation of plausibility and belief within each interval “cell”
  - Easily parallelized.

Original LHS samples used to generate a surrogate.

Million sample points generated from the surrogate, used to determine the max and min in each “cell” to calculate plausibility and belief.
Bayesian Analysis

• Construct a prior distribution on a parameter (which might be a parameter of a distribution)
• The prior distribution should be based on previous experience, engineering judgment
• The distribution on the prior is updated with actual data. The resulting updated distribution is called the posterior.

<table>
<thead>
<tr>
<th>Frequentist</th>
<th>Bayesian</th>
</tr>
</thead>
<tbody>
<tr>
<td>Assumes there is an unknown but fixed parameter $\theta$</td>
<td>Assumes a distribution on unknown parameter $\theta$</td>
</tr>
<tr>
<td>Estimates $\theta$ with some confidence interval</td>
<td>Uses probability theory, treats $\theta$ as a random variable</td>
</tr>
</tbody>
</table>
Bayesian Analysis

• Why would we use it for CS&E problems?
• Nice feature of incorporating additional data as it becomes available
• We often don’t have good estimates: Bayes provides a framework for starting with what we do know, and refining our estimates in a statistically consistent manner
• Examples:
  – Reliability problems: Update probability of failure
  – Response surfaces: Update parameters in a surrogate model for a trust region
  – Calibration under Uncertainty (CUU): Update our parameter estimates based on experimental data AND uncertainty in a model
Bayesian Methods

Discrete Case

\[
p(\theta \mid x) = \frac{p(x, \theta)}{p(x)} = \frac{p(x \mid \theta) p(\theta)}{p(x)} = \frac{p(x \mid \theta) p(\theta)}{\sum_{\theta} p(x \mid \theta) p(\theta)}
\]

where \( \theta \) is a parameter(s), \( x \) is a data vector, and \( p \) is a probability mass function.

\[
p(\theta \mid x) = \text{posterior} \propto p(x \mid \theta) p(\theta) = \text{likelihood} * \text{prior}
\]
Examples

- Use Binomial distribution to model the number of failures, \( x \), in \( n \) trials.

\[
f(x \mid \theta) = \binom{n}{x} \theta^x (1 - \theta)^{n-x}
\]

- We obtain data that shows 2 failures in 5 trials

<table>
<thead>
<tr>
<th>Prior Probability</th>
<th>Posterior Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P{\theta=0.3}=0.1 )</td>
<td>( P{\theta=0.3}=0.13 )</td>
</tr>
<tr>
<td>( P{\theta=0.6}=0.9 )</td>
<td>( P{\theta=0.6}=0.87 )</td>
</tr>
</tbody>
</table>

- The posterior distribution reflects the fact that in this set of data, \( \theta = 0.4 \) which is closer to 0.3 than 0.6 and so the probability of \( \theta=0.3 \) has risen slightly.