Validation & Verification and Uncertainty Quantification at Sandia

Brian M. Adams
Sandia National Laboratories
Optimization and Uncertainty Quantification

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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.
To be credible, simulations must be verified, validated with data, and deliver a best estimate of performance, together with its degree of variability or uncertainty.

- Credible simulation and V&V
- Characterizing and propagating uncertainty for risk analysis and validation
- Intro to aleatory and epistemic UQ in DAKOTA
- Application examples:
  - UQ for CMOS7 ViArray UQ
  - Sandia’s QASPR program: computational model-based system qualification

Slide credits: Mike Eldred, Laura Swiler, Tony Giunta, 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
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
Credible Simulation: V&V and UQ

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

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Verification & Validation

• Ultimately, quantification of margins and uncertainties (QMU): How close are my uncertainty-aware code predictions to required performance?

• 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; relies on uncertainty quantification (UQ)

• Verification: “Are we solving the equations correctly?”
  – A mathematics/computer science issue: is our mathematical formulation and software implementation of the physics model correct?
  – code verification (software correctness): SQE, especially unit/regression/verification testing; analytic problems, method of manufactured solutions
  – solution verification: e.g., exhibits proper order of spatial/temporal/iterative convergence. Algorithms: Richardson extrapolation, finite element error estimation (ZZ, QOI)

\[
p = \frac{1}{\ln r} \ln \left( \frac{E_{\text{grid} 1}}{E_{\text{grid} 2}} \right)
\]

\[
\eta^2 \equiv \int_{\Omega} T(u_h) : (\nabla z_h - \nabla z_h) \, d\Omega
\]
Algorithms for Computational Modeling & Simulation

Are you sure you don’t need verification?!

Optimization and UQ

Adapt

Time integration

Nonlinear solve

Linear solve

Information Analysis & Validation

Improved design and understanding
Hierarchical Validation Experiments
(Abnormal Thermal Environment)

Validation: “Are we solving the right equations?” Based on experimental data and metrics, is the model sufficient for the intended application?

Increasing complexity, fewer experiments

Deployed System

Full System

Subassemblies

Components

Separable Effects

Bill Oberkampf
Validation Metrics: Quantitative Comparison with Experiment

(a) Viewgraph Norm  
(b) Deterministic  
(c) Experimental Uncertainty  
(d) Numerical Error  
(e) Nondeterministic Computation  
(f) Statistical Comparison

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Validation Metrics: Quantitative Comparison with Experiment

(a) Viewgraph

(b) Final Temperature Values

(c) Experimental Uncertainty

(d) Numerical Error

(e) Nondeterministic Computation

(f) Statistical Comparison

Bill Oberkampf
Extrapolating Beyond Validation Domain
Uncertainties to Quantify

A partial list of uncertainties affecting computational model results

• **typical parametric uncertainty**, incl. random fields/processes
  – physics/science parameters
  – statistical variation, inherent randomness
  – operating environment, interference
  – initial, boundary conditions; forcing
  – geometry / structure / connectivity
  – material properties
  – manufacturing quality

• **model form / accuracy**

• **program**: requirements, technical readiness levels

• **human reliability**, subjective judgment, linguistic imprecision

• **numerical accuracy**: mesh, solver, approximation error

• **experimental error**: measurement error, bias
Why Uncertainty Quantification?

• 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
Verification & Validation: A Formal, Iterative Process

- **Validation** is “the process of determining the degree to which a computer model is an accurate representation of the real world from the perspective of the intended model applications.”

- Relies on comparing code calculations to results of physical experiments, with the goal of developing and quantifying confidence in codes to predict a specified problem result.

- Credibility assesses model and experiment relevance, quantification and capture of non-deterministic components, and model adequacy.

Well-characterized result: BEST ESTIMATE + UNCERTAINTY

Trucano et al; SAND Report 2002-0341
Coverage Matrix Shows Code Features Exercised in Verification Tests

Matrix helps prioritize gaps, create new verification problems to fill most important, w.r.t. intended use.
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

- 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
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

**Final Temperature Values**

<table>
<thead>
<tr>
<th>Temperature [deg C]</th>
<th>% in Bin</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0</td>
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<tr>
<td>36</td>
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<td>78</td>
<td>2</td>
</tr>
<tr>
<td>84</td>
<td>1</td>
</tr>
</tbody>
</table>

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
- \( \text{Mean}(T), \text{StdDev}(T), \text{Probability}(T \geq T_{\text{critical}}) \)
UQ: Sampling Methods

Given distributions of $u_1, \ldots, u_N$, UQ methods...

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

Output Distributions

...calculate statistical info on outputs $T(u_1, \ldots, u_N)$

Final Temperature Values

Temeprature [deg C]

% in Bin

30 36 42 48 54 60 66 72 78 84
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.
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

Upcoming (Mike): DAKOTA enables more efficient UQ by combining optimization, uncertainty analysis methods, and surrogate (meta-) modeling in a single framework.
Challenge: Epistemic UQ

- **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

<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>
Propagating 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
Use DAKOTA with Xyce circuit simulator to perform pre-fabrication uncertainty analysis of new CMOS7 ViArray

- ViArray: generic ASIC implementation platform
- Target applications: guidance, satellite, command & control
- Assess voltage droop/spike during photocurrent event
- Consider effect of process variation in each ‘layer’ on supply voltages; representative distributions:
  - Truncated normals used for METAL and VIA; truncated lognormals used for CONTACT and polyc.
ViArray: Benefits of UQ

- One ensemble of UQ calculations used to determine most sensitive parameters and output ranges: determined that sensitivity depends on final chip configuration

- Suspicious UQ results led to correcting simulation failures not observed at nominal parameters

- Gave process engineers and circuit designers insight into possible circuit behaviors

- Sensitivity could help guide data collection

- Ongoing work: assess interaction of package parasitics with on-chip parasitics, V&V for photocurrent generation models
Neutron Radiation Exposure Degrades Electronics

- Military requirement: certify to hostile environment

- Neutrons create damage

- Damage degrades gain

- Prerad: $\beta_0 = 150$
• Military requirement: certify to hostile environment
• SPR dismantled end of FY06 to improve security posture
Neutron Radiation Exposure Degrades Electronics

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QASPR (Qualification Alternatives to Sandia Pulse Reactor) methodology will certify qualification via modeling & simulation with quantified uncertainty
QASPR: Science-Based Engineering Methodology For Qualification

Risk Informed Decisions

Qualification Evidence

select experiments in alternate facilities

γ,n – 100 ms long pulse
ion – 100 μs short pulse

uncertainty quantification

high performance, multi-fidelity, predictive computational modeling

validation
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)

- peak damage
- +2σ
- -2σ

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

- Fairchild response data within SPR hidden
- First *prototype* of the QASPR methodology (and real validation of the QASPR system)
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UQ algorithms have a critical role in system validation

Transient Device Damage Response
SPR 13267q1 (black) and Simulation bounds (yellow)

+/- 1-2% vertical error on experimental measurement
Model Validation: Blind Prediction

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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**

- **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)

- **sub-circuit: 10s to 100s of devices**

- **ASIC: 1000s to millions of devices**

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

To be credible, simulations must be verified, validated with data, and deliver a best estimate of performance, together with its degree of variability or uncertainty.

• Formal V&V process helps certify credible simulation

• Uncertainty quantification algorithms are essential in validation and calibration under uncertainty

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

Thank you for your attention!

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