V&V, UQ, and Predictive Science Challenges in the ASC and PSAAP Programs

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Outline

• SNL V&V program overview

• SNL research interests

• Technical/programmatic challenges in the PSAAP program

• Summary
NNSA/Sandia Have Policies on QMU Deployment

• NNSA draft policy (May 2007):

  *Nuclear Weapon Assessments Using Quantification of Margins and Uncertainties Methodologies:*
  “Design agency assessments shall incorporate QMU methodologies as an essential part of the framework necessary for the evaluation of the performance of warhead and warhead components.”

• Sandia directive (April 2007):
  Steve Rottler, Vice President of Sandia Weapon Engineering:
  “We explicitly account for, monitor, and analyze margins and uncertainties throughout the warhead lifecycle using tools and a methodology collectively referred to as the Quantification of Margins and Uncertainties.”

• Also have historical weapon qualification requirements:
  – Probability of inadvertent nuclear detonation < 1x10^-m for normal environments.
  – Probability of inadvertent nuclear detonation < 1x10^-n for abnormal environments.
Sandia is Using V&V/UQ/QMU in Annual Stockpile Assessments

• Sandia is now applying modeling/simulation-based QMU to some attribute/environment of every nuclear weapon in the US stockpile.
  – We are working with our colleagues in weapon engineering and weapon safety to identify and address the most critical weapon and scenario combinations.

• Goal – make statements such as the following:

  “We are ###.#% confident that the probability of failure in [Scenario A] for [Weapon B] is less than 1x10^{−n}.”

  and

  “Here is a peer-reviewed ‘evidence package’ to back up that statement.”

• We are already doing this, but it is not yet routine work:
  – Weapon #1: abnormal mechanical (drop impact) QMU with 33 high fidelity SIERRA simulations
    • ~1M CPU hours on Red Storm, total
  – Weapon #2: abnormal thermal (fuel fire) QMU with 60 high fidelity SIERRA simulations.
  – New application: abnormal mechanical QMU with ~10 high fidelity SIERRA simulations
    • ~4M CPU hours on Red Storm, total (when completed)
Sandia’s Applications Span Diverse Physics and Wide Spatial and Temporal Scales

• Solid Mechanics:
  – Vehicle (truck, weapon) crash simulations with plastic deformation and multiple contacts
  – Multiscale: 10’s of meters (e.g. loads transferred through vehicle) down to microscale (metal component failure)

• Thermal/Fluid Mechanics:
  – Vehicle (truck, aircraft, rocket) accident with burning fuel
  – Multiscale: 10’s of meters (vehicle & flame size) down to microscale (foam decomposition rates/products, propellant burn)

• Coupled crash & burn simulations – same issues as above two

• Re-entry Effects:
  – Hypervelocity flows with shocks, ablation, and random pressure fields
  – Explosive blast loading with nonlinear energy dissipation in joints
  – Multiscale: vehicle length is O(1m), relevant physics at microscale

• Radiation Effects:
  – Vehicle irradiation both short & long term
  – Multiscale: 10’s-100’s of meters (radiation transport) down to nanoscale (atomic lattice displacements)
V&V/UQ/QMU Thinking is Embedded in Sandia’s QASPR Project

• **Purpose:** Qualify electrical components for radiation environments.

• **Goal:** Predict, with quantified uncertainty, electrical component response in radiation environments *using simulations & test facilities.*

• **Approach:**
  – Obtain relevant radiation effects data from existing test facilities (ion beams, electrons, gamma rays, neutrons, etc.)
  – “Atoms-to-circuits” modeling and simulation activity across SNL organizations
  – Quantify uncertainty in test data & simulation data; validate computer models
  – Apply QMU methods to assess electrical device performance vs. requirements.

Radiation Env: x-rays, gamma rays, neutrons, etc.

Atomic-scale defects

Device effects (transistor, diode, etc.)

Circuit effects

QMU Assessment
Sandia Has Developed, and is Deploying, a Disciplined V&V Process

1. DP Application
2. Planning
3. Code Verification
4. Experiment Design, Execution & Analysis
5. Metrics
6. Assessment
7. Prediction & Credibility
8. Document

- Understand the application and requirements
- Assess capabilities, identify gaps, & prioritize work
- Compare to test data
- Predictions w/ quantified uncertainty
- Convergence checks on engineering application
- Software quality practices & numerical accuracy checks on test problems
- Calculation Verification
- Validation Experiment Centered Elements

...
What’s New in Sandia’s V&V/UQ/QMU?

• Software tools evolving:
  – *DAKOTA*: optimization, uncertainty quantification and sensitivity analysis software tool kit
    • includes extensive polynomial chaos capabilities (nonintrusive)
  – *Encore*: error estimation and finite element mesh adaptivity
    • automatic mesh doubling for complex geometries

• VV/UQ/QMU implementation evolving:
  – PCMM – predictive capability maturity model developed by Pilch, et al.
  – Goal: provide a means to assess and communicate evidence supporting credibility of simulations.
### Predictive Capability Maturity Model (PCMM)

**Measures and Communicates Maturity of Mod/Sim Process**

<table>
<thead>
<tr>
<th>PREDICTIVE ATTRIBUTE</th>
<th>Level 0</th>
<th>Level 1</th>
<th>Level 2</th>
<th>Level 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low-Consequence M&amp;S-Informed, e.g., Scoping or Res Activities</td>
<td>Score=0</td>
<td>Score=2</td>
<td>Score=4</td>
<td>Score=6</td>
</tr>
<tr>
<td>Low-Consequence M&amp;S-Informed, e.g., Design Support</td>
<td>Score=2</td>
<td>Score=4</td>
<td>Score=6</td>
<td></td>
</tr>
<tr>
<td>High-Consequence M&amp;S-Informed, e.g., Qualification Support, Score=4</td>
<td>Score=6</td>
<td></td>
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</tr>
<tr>
<td>High-Consequence M&amp;S-Based, e.g., Qualification Support</td>
<td>Score=6</td>
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</table>

- **Key issues:**
  - **Horizontal Axis** – measures level of rigor in a mod/sim activity.
  - **Vertical Axis** – covers different aspects of mod/sim activity (geometric fidelity, physics fidelity, verification, validation, UQ, etc.).
  - **PCMM provides a means to consistently document and communicate the status of a complex VV/UQ/QMU study to a non-ASC weapons customer.**
  - **Peer review is a critical component of PCMM (above level 0).**
Sandia has an Active VV/UQ/QMU Research Program

• Verification:
  – Method of manufactured solutions and related approaches
  – Error estimation methods

• Validation:
  – Bayesian methods for hierarchical validation
  – Uncertainty extrapolation methods outside of validation domain

• Uncertainty Quantification:
  – more efficient sampling methods for propagating aleatory and epistemic uncertainty
  – “embedded” UQ methods in physics simulation codes
  – surrogate-based UQ using a combination of low and high fidelity physics models
    • surrogate = reduced order physics model, simplified geometry model, coarse mesh model, response surface model, etc.
Opportunities in the ASC/PSAAP Partnership

• Technical:
  – Collaborations on new V&V/UQ/QMU methods.
    • Common demonstration problems?
  – Collaborations on error estimation methods.
    • What engineering problems can/cannot be addressed with current methods? What should we be doing next?
  – Collaborations on code development.
    • “Embedded UQ” methods, and, methods for new computer architectures.

• Programmatic:
  – Tri-labs and PSAAP schools should meet early and often.
    • workshops, informal visits, etc.
  – We’re looking for students (& future hires) who are broad and deep.
    • The PSAAP educational/collaboration plans appear to be aimed in this direction.
Summary

• Past ~10 years have laid out the groundwork for V&V, UQ, QMU methods.
  – Research on innovative math/statistical methods at Tri-Labs and ASCI Alliance schools.
  – Development of key software tools:
    • At Sandia - DAKOTA, Encore, SIERRA, RAMSES, etc.
  – Demonstrations on key weapon projects.

• Going forward:
  – Continuing vigorous V&V/UQ research program.
  – Deploying V&V/UQ methods to the Sandia analyst community.
  – Socializing V&V/UQ issues with weapon engineering managers.
  – Supporting annual weapon stockpile assessments.
  – Collaborating with universities (PSAAP, etc.) to improve the technical basis for our V&V/UQ/QMU methods.
Points of Contact

• Tony Giunta’s contact info:
  – Phone: 505/844-4280
  – Email: aagiunt@sandia.gov
What’s New in Sandia’s VV-UQ-QMU?

• 1996-2006:
  – V&V, UQ, QMU methods evolving
  – V&V, UQ, QMU applied on major milestones, but not in everyday work.
  – Software tools evolving:
    • DAKOTA – uncertainty quantification and sensitivity analysis.
    • Encore – error estimation and finite element mesh adaptivity.

• 2007-Present:
  – PCMM – predictive capability maturity model developed by Pilch, et al.
  – Goal: provide a means to assess and communicate evidence supporting credibility of simulations.
  – Stress practical VV-UQ-QMU, training, and teaming
Verification, Validation, and Uncertainty Quantification are the Science Behind QMU

• Verification – “Are we solving the equations correctly?”
  – Correctness of implemented mathematical algorithms.
  – Convergence to the answer at correct rate for problems w/ known solns.
  – Convergence to an answer for complex problems w/o known solns.

• Validation – “Are we solving the right equations?”
  – Correctness of physical models and sufficiency for the application.

• Uncertainty Quantification (UQ):
  – Statistical propagation of uncertainty through a simulation model, and statistical interpretation of model response.
    • Key issue: distinction between aleatory (probabilistic) and epistemic (lack of knowledge) uncertainties in UQ, and, their correct mathematical propagation (leveraging Waste Isolation Pilot Plant UQ work)

• Interpolation / Extrapolation and QMU:
  – Application of the simulation model to untested physical regimes, with quantified uncertainty on predictions (math + stats + physics).
Typical QMU Application

Motivation:
• US weapons must survive a harsh shock and vibration environment en route to target.

Example:
• max acceleration load is “k”.
• weapon designed to withstand acceleration load of “m” (m>k).

QMU Issues:
• Difference between “m” and “k” is the margin.
• There is usually uncertainty around “m” and sometimes around “k”.
• System engineers track k, m, m’s uncertainty, m’s change with time.
• Engineering analysts perform the calculations that produce the knowledge about “m”.
  • Typical approach: find worst case “m” vs. “k” (i.e., worst-case margin).
  • QMU approach: quantify margin & uncertainty for “m” vs. “k”.

Tactical Environment
Complex Shock & Vibration Environment on Re-entry
Predictive Capability Maturity Model: Example Self-Assessment (Goal is Level 2)

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</thead>
<tbody>
<tr>
<td><strong>Representation or Geometry Fidelity</strong>&lt;br&gt;Are you overlooking important effects because of defeaturing or stylization?</td>
<td>Grossly defeatured or stylized representation based on judgment or practical considerations</td>
<td>Significant defeatureing or stylization based on judgment or practical considerations or lower fidelity representation justified w/ a significantly defeatured or stylized representation</td>
<td>Limited defeatureing or stylization judged to retain the essential elements of “as built” or appropriate lower fidelity representation justified w/ a slightly defeatured or stylized representation</td>
<td>Highest fidelity representation “as is” w/o sig defeaturing or stylization or appropriate lower fidelity representation justified w highest fidelity representation</td>
</tr>
<tr>
<td><strong>Physics and Material Model Fidelity</strong>&lt;br&gt;How science-based are the models?</td>
<td>Unknown model form represented with ad hoc knob non-uniquely calibrated to IET</td>
<td>Empirical model applied w/ significant extrapolation, uniquely calibrated with IET</td>
<td>Physics informed models applied w/ significant extrapolation, unique calibrations with SET</td>
<td>Well accepted physics-based model applied w/ significant extrapolation</td>
</tr>
<tr>
<td><strong>Code Verification</strong>&lt;br&gt;Are software errors or algorithm deficiencies corrupting simulation results?</td>
<td>Judgment only</td>
<td>Code managed to SQE standards Sustained unit/regression testing w/ significant coverage of required Features and Capabilities (F&amp;Cs)</td>
<td>Code managed and assessed (internally) against SQE standards Sustained verification test suite w/ significant coverage of required F&amp;Cs</td>
<td>Code managed and assessed (externally) against SQE standards Sustained verification test suite w/ significant coverage of required F&amp;Cs and their interactions</td>
</tr>
<tr>
<td><strong>Solution Verification</strong>&lt;br&gt;Are numerical errors corrupting simulation results?</td>
<td>Judgment only Sensitivity to discretization and algorithm parameters explored in SRQs not directly related to the decision context</td>
<td>Sensitivity to discretization and algorithm parameters explored w/ significant coverage of required SRQs directly related to the decision context Numerical errors estimated in SRQs not directly related to decision context</td>
<td>Numerical errors estimated in SRQs directly related to the decision context Rigorous numerical error bounds quantified in SRQs directly related to the decision context</td>
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</tr>
<tr>
<td><strong>Validation</strong>&lt;br&gt;How accurate are the models?</td>
<td>Judgment only Qualitative accuracy w/o significant SET coverage Quantitative accuracy w/ assessment of unc and w/o significant SET coverage</td>
<td>Quantitative accuracy w/ significant SET coverage w significant SET coverage and IETs</td>
<td>Quantitative accuracy w/ significant SET coverage and IETs</td>
<td>Quantitative accuracy w assessment of unc</td>
</tr>
<tr>
<td><strong>UQ and Sensitivities</strong>&lt;br&gt;What is the impact of variabilities and uncertainties on performance and margins?</td>
<td>Judgment only Deterministic assessment of margins (e.g., bounding analyses) Informal “what if” assessments of unc, margins, and sensitivity Aleatory and epistemic uncertainties represented and propagated w/o distinction Sensitivity to uncertainties explored</td>
<td>Aleatory and/or epistemic uncertainties represented separately and propagated w significant strong assumptions Quantitative sensitivity analysis w/ significant strong assumptions Sensitivity to numerical errors explored</td>
<td>Aleatory and/or epistemic uncertainties represented separately and propagated w/ significant strong assumptions Quantitative sensitivity analysis w/ significant strong assumptions Sensitivity to numerical errors explored</td>
<td>Aleatory and/or epistemic uncertainties represented separately and propagated w/ significant strong assumptions Quantitative sensitivity analysis w/ significant strong assumptions Numerical errors quantified</td>
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Sandia VV/UQ/QMU Status: July 2008

• FY08 ASC V&V Program:
  – Emphasis on “practical VV/UQ/QMU”
  – Trial use of PCMM on all V&V-funded projects.
  – Training offered:
    • V&V 2-day short course, QMU 1-day workshop (trained 100+ staff)
    • VV/UQ/QMU seminars held ~every 3 weeks (~350 attendees, 10 seminars)
  – In the works:
    • Engaging ASC SIERRA and RAMSES code development teams on “practical verification” steps.
    • “Practical validation” ½ day workshop to be given in August’08

• FY09 ASC V&V Program:
  – PCMM table as the framework for planning and communicating VV/UQ/QMU elements of each project
  – Will provide VV/UQ/QMU “best practices” to ASC PIs and teams.
  – Will require VV/UQ/QMU plan document by Q1FY08 for all projects, and, will be reviewed by managers/peers.
  – Continued emphasis on practical VV/UQ/QMU approaches.
Predictions w/ Quantified Uncertainty

- QMU: Use simulations, and quantified uncertainties, for performance predictions and margin estimates at untested conditions. – via DAKOTA
  - And, assess adequacy of margin in electrical device performance

Estimate: probability gain < critical_gain, and Margin/Uncert.
Predictions w/ Quantified Uncertainty

Estimate: probability that safety system fails, and Margin/Uncert.