SAND2010-1935P

Overview of Verification, Validation, Uncertainty Quantification, and QMU

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Outline

- Introduction
- Background on:
  - Verification & Validation (V&V)
  - Quantification of Margins and Uncertainties (QMU)
- Engineering Application
- V&V at Sandia Today
- Predictive Capability Maturity Model (PCMM)
- Summary

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- **Introduction**
- **Background on:**
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  - **Quantification of Margins and Uncertainties (QMU)**
- **Engineering Application**
- **V&V at Sandia Today**
- **Predictive Capability Maturity Model (PCMM)**
- **Summary**

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Introduction

- **Our common ground:**
  - **The nation is making million/billion $ decisions that are strongly influenced by computational simulation – e.g., weapon life extensions, full scale tests, facility/infrastructure protection upgrades, etc.**
  - **How do we build/demonstrate confidence in our comp. sim. results?**
  - **How do we communicate margins and uncertainties to decision makers?**

- **My goals for this talk:**
  - **Influence your thinking about computational simulation, via role of:**
    - **verification & validation (V&V)**
    - **sensitivity analysis and uncertainty quantification (UQ)**
    - **quantification of margins and uncertainties (QMU)**
  - **Describe some of Sandia's current efforts where comp. sim. was employed along with V&V/UQ/QMU practices.**
  - **Motivate you to attend all classes in ESP700.**

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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 correct answer, at the correct rate, as model is refined.
- **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.
- **Quantification of Margins and Uncertainties (QMU):**
  - Using the simulation model to make system performance predictions with quantified uncertainty, and with quantified margins with respect to system performance requirements.

V&V Is a Tough Sell

- **V&V is expected, but not well understood, by decision makers.**
  - **V&V is, in a nutshell, all about putting "correct" math methods and physics models in our codes.**
  - **We're expected to produce "correct" codes.**
  - **"If you haven't been doing V&V all along, then what have you been doing with my _____ money?"**

- **What's different now?**
  - **Computational simulation is different now than 10-20-30 years ago (e.g., auto industry, aircraft industry, nuclear weapons industry)**
    - **We're making million/billion $ decisions that are heavily influenced by comp. sim.**
  - **Definition of "correct codes/models" (see above) is now changing.**
  - **"Before I spend $M/$B on a decision, I want evidence of the correctness of your comp. sim. model and results."**

- **Issues: Code correctness is expected, quantified evidence of correctness (via V&V) takes extra effort beyond traditional code development work, you can't V&V every aspect of a code/model/project, and it's hard to retrofit V&V into a study that is already completed.**

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What Does Sell?

- Using comp. sim. results to aid decision making sells.
  - Decision making is based on knowing the tradeoffs for competing objectives, due to variations in designer-controllable parameters.
  - Quantities of interest: cost & performance
  - This sells (re: facility design hardness study):
    - "If you increase factor1 by A% and lower factor2 by B%, you reduce cost by X% and decrease the probability of kill by Y%."
    - "By the way, here is the evidence (tucked away in a report appendix) for the validity of predictions A, B, X, and Y."
  - This also sells:
    - "If were going to perform a comp. sim. study that influences a $M/$B decision, then let's carve out $m to run a V&V study to make sure we're getting good data, and $n to perform an adequate sensitivity/uncertainty analysis."

- Punch Line:
  - V&V doesn't sell for it's own sake.
    - Decision makers don't care about the rate of convergence of an iterative mathematical method, or % line coverage of tests.
    - For $M/$B issues, decision makers do care that you got the right answer and they expect a technical pedigree (aka "provenance") for your work.
  - V&V sells when it is included as an aid to decision making.
    - i.e., when V&V provides supporting evidence (provenance) to sensitivity analysis and UQ results on relevant technical/financial issues.

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Sandia's QMU Methods Have Roots in Nuclear Reactor Safety & Waste Storage

- Circa 1992: National decision to cease nuclear testing.
- Circa 1996: DOE establishes stockpile stewardship program.
  - Accelerated Strategic Computing Initiative (ASCI)
  - Advanced Simulation and Computing (ASC) Program
- Circa 1999: ASCI Verification and Validation (V&V) program started.
  - Key technical link: Jon Helton – led V&V/QMU effort for Waste Isolation Pilot Plant (WIPP) risk assessment & now consultant to SNL V&V Program
  - e.g., WIPP repository: US EPA has probability-based limits on release of radioactive waste to environment for 10,000 years
  - WIPP had: (a) physics-based, test data-vetted computational models, (b) ability to handle uncertain/probabilistic conditions and parameters, and (c) ability to make defensible performance predictions out to a long-term time horizon, subject to a National Academy level of peer review.
- 2003-Today: ASC program staff applying V&V/QMU practices in stockpile assessment studies; collaborating with others across Sandia.

QMU methods are used for weapon applications, however, QMU methods are still evolving.

What is QMU?

- **QMU: Quantification of Margins and Uncertainties**
  - **Margin - Difference between system's nominal/median performance vs. a do-not-exceed threshold.**

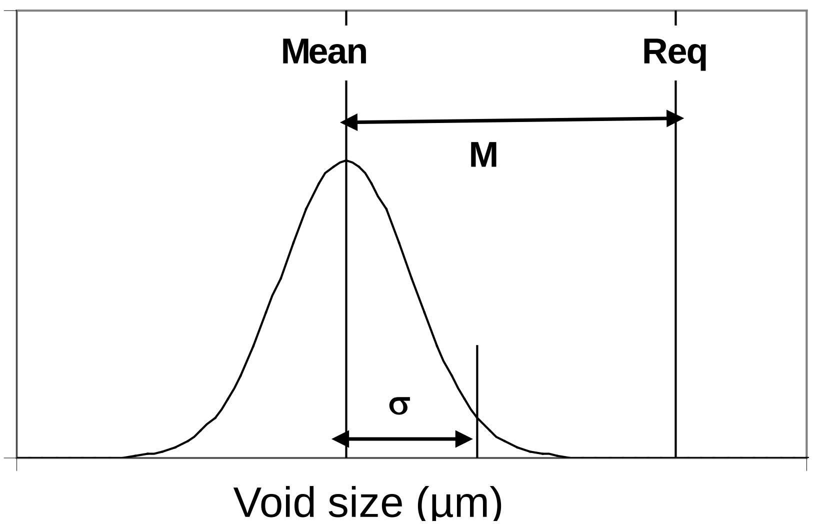
- **Sandia is employing QMU to:**
  - **Understand performance margins, uncertainties, & changes with time.**
  - **Provide higher confidence that our products meet requirements.**

- **NNSA and DoD customers have statistics-based requirements:**
  - **Probability of an Inadvertent Nuclear Detonation < $1x10^{-m}$ for normal environments.**
  - **Probability of an Inadvertent Nuclear Detonation < $1x10^{-n}$ for abnormal environments.**
    - **What is the probability of a welded joint failure if weapon Wxx is dropped from *k* feet?**

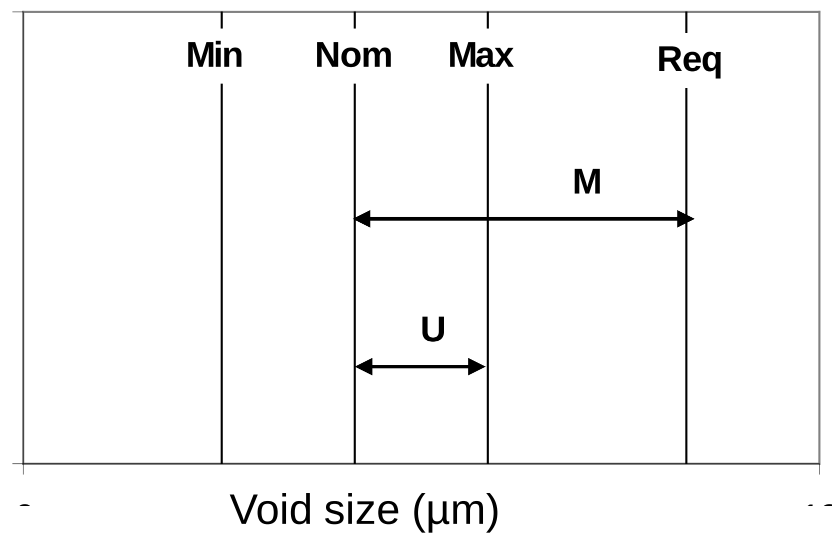
- **To answer these questions we need data ensembles:**
  - **Test data (both historical and new).**
  - **Simulation data (both medium- and high-fidelity).**

QMU Methods: A Quick Overview

Aleatory (Probabilistic) Uncertainties



Epistemic (Lack of Knowledge) Uncertainties



Hypothetical Example #1:

- Probability distribution curve obtained from many samples of void size in a material.
- "Req" = do-not-exceed void size.
- Margin (M), Standard Deviation (σ)
- M/σ is called the "k-factor"
- Can estimate Probability(void size > Req) and track M/σ changes w.r.t. time.

Hypothetical Example #2:

- Insufficient data to specify a probability distribution – only know min & max void size.
- Margin (M), Uncertainty (U)
- M/U is the "confidence ratio"
- Cannot estimate Prob(void size > Req), but can track M/U w.r.t. time.

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How Does QMU at Sandia Compare to Approaches Used in Industry?

- My view:
  - QMU is the SNL/LANL/LLNL approach that inserts “statistical thinking” into engineering practice.

- “Statistical thinking” is now common in engineering and business practice:
  - Design for Six Sigma / Lean Six Sigma:
    - General Electric, Motorola, Honeywell, Raytheon, Caterpillar, Bank of America, Merrill Lynch, etc.
  - Robust design (aka Taguchi methods):
    - Japan & US auto industry

- Some US Government organizations have a tradition of probabilistic requirements, assessments, and regulations:
  - US Nuclear Regulatory Commission
  - US Environmental Protection Agency
  - NNSA

NNSA and Sandia Now 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."**

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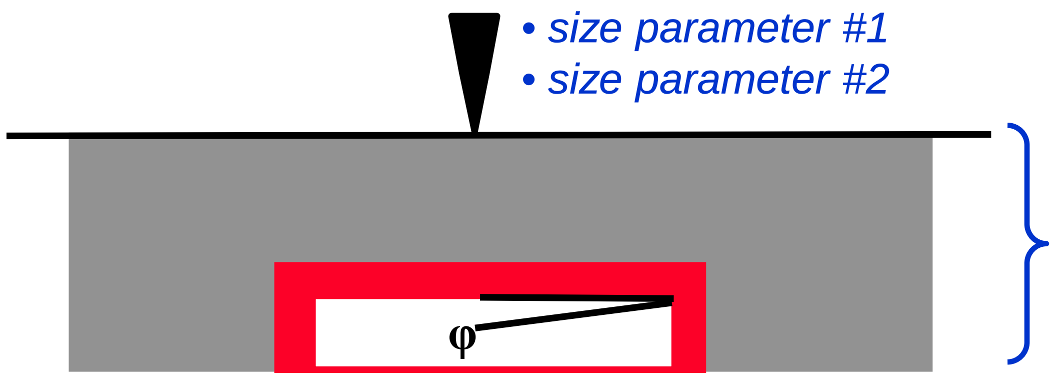
Example:
Underground Target Defeat/Protect Study

- **<u>Scenario</u>: underground target subject to an external threat**
- **<u>Goal</u>: Assess sensitivity/uncertainty in target response due to uncertainties in target construction and threat characteristics**
- **<u>Approach</u>: 9 parameters define uncertainties in threat and target**
  - **Each parameter has uncertainty specified by an interval**
- **<u>Metric</u>: deflection angle (φ) of target roof at mid-span (>critical angle=kill)**
- **<u>Tools</u>: CTH, DAKOTA, JMP statistical analysis software**

<u>Threat:</u>
- *size parameter #1*
- *size parameter #2*



<u>Target:</u>
- *Soil depth*
- *Materials*
- *Dimensions of structure – height, width, thickness, etc.*

<u>What Matters?</u>:
<u>Defense</u>: What design features (and how much $) are needed to protect my facility?
<u>Offense</u>: What facilities can I hold at risk, given my range of threat assets? What different assets (w/ different costs) I can employ to have high kill probability, given uncertainty in the target composition?

We Took a Nontraditional Approach in this Study, But Did Not Use V&V Best Practices

- **Traditional approach:**
  - **Build computational model**
  - **Perform a user-guided sequence of "change one parameter at a time" runs of the computational model (~20-50 runs total - estimated)**
  - **Payoff: develop qualitative/quantitative parameter sensitivity and trend information for facility response (roof deflection) vs. 9 parameters**
    - **generate "local" performance information that looks like a derivative: e.g. d(deflection angle)/d(soil depth), etc.**

- **Nontraditional approach with sensitivity/uncertainty quantification:**
  - **Build computational model**
  - **Use statistical data sampling methods to develop a "code run matrix" (initially 50 runs; 150 runs total); then run the code**
  - **Use statistical data analysis tools to sift the data**
  - **Payoff: (a) identify & quantify influence of 9 parameters, (b) produce global trend (tradeoff) models of facility response (roof deflection) vs. variations in the 9 parameters**
    - **you get quantified single- and multi-parameter sensitivity information**
    - **you get local and global tradeoff information**
  - **Repeat with new run matrix, if needed.**
  - **Cost: (a) one or more folks on the team need to know how to do the statistical sampling & analysis (training), (b) # code runs >= than traditional approach (% increase is problem dependant)**

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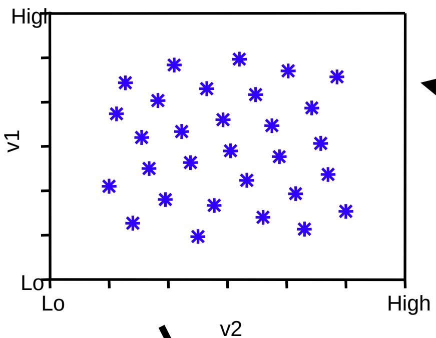
Example Study: Underground Target Defeat/Protect

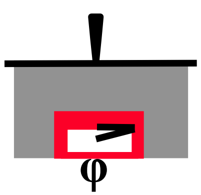
- **Example: Sensitivity analysis study with CTH and DAKOTA; simulations run on a Linux cluster; data analysis via JMP commercial statistics package**

Statistics-based "run matrix"



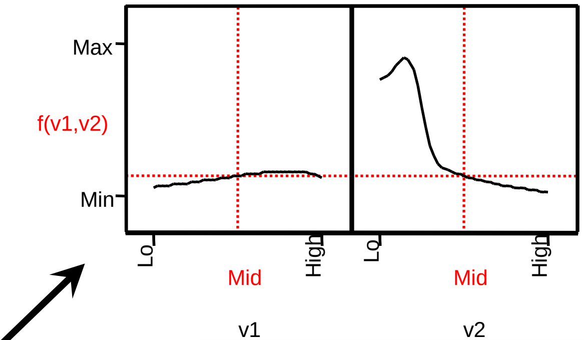
DAKOTA

CTH sims. run on a LINUX cluster



JMP
The Statistical Discovery Software

Graphics



Statistical analysis

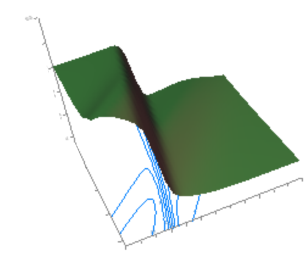
Summary of Fit

RSquare	0.866299
RSquare Adj	0.823758
Root Mean Square Error	#.#
Mean of Response	#.#
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	7	5343.9158	763.417	20.3638
Error	22	824.7562	37.489	Prob > F
C. Total	29	6168.6720		<.0001

Yields Qualitative and Quantitative Insight, e.g.:
- *Most important parameters*
- *Cost & Survivability tradeoff functions vs. parameter variations*



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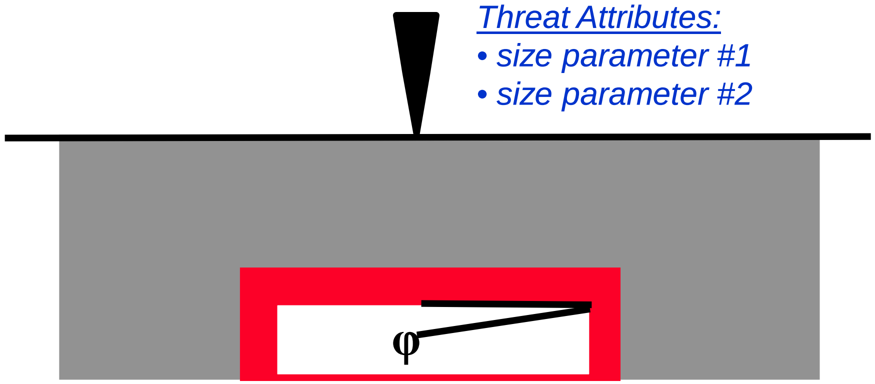
Sensitivity Analysis and UQ Study: Underground Target Defeat/Protect

<u>Results</u>:
- Identified 3 key target design attributes that most strongly affect facility cost & performance.

- Generated a statistical/mathematical model of roof deflection vs. 9 parameters -- useful as a planning tool for SNL and customer in considering various design tradeoff studies.

- Influenced the design of an expensive, large scale test.



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Where was V&V in this Study?

- Little/no formal V&V; some "historical" V&V.
  - Verification: some test problems with analytical solutions probably in the code test suite
  - Validation: considerable user experience, plus, broad testing of this code in Sandia/external community
  - Note: This study was done ~6 years ago.

- What would we do differently now?
  - Verification #1: Identify a few key analytic test problems to confirm that the code converges to (a) the right answer, and (b) at the right spatial/temporal rate.
  - Validation: Identify a few key experimental test data sets and confirm that "test data + uncertainty" and "sim data + uncertainty" agree sufficiently.
  - Verification #2: Perform some basic mesh convergence studies with the threat/target geometry to (a) confirm that the mesh is sufficiently refined that the results are converging to <u>an</u> answer, or (b) inform us that the mesh is not converged and that we need to be wary of the sensitivity/UQ results.

- Why would we do this extra work?
  - In almost every major V&V study that we've done, we found one or more serious errors in the math (numerics) and/or physics.
    - Best case – the code still converges to the right answer, slower than it should
    - Worst case #1 – the code doesn't converge to any answer
    - Worst case #2 – the code converges to the wrong answer, slowly

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Where is Sandia Now w.r.t. V&V?

- SNL nuclear weapon mission drivers:
  - annual assessment & certification that all weapon types are safe, secure & reliable

- Few/no tests at the full system level; few/some/no tests at subsystem/component level:
  - not allowed, and/or (radiation effects tests)
  - too expensive, and/or (crash impact tests)
  - too environmentally unfriendly, and/or (fuel/propellant fire tests)
  - too few units available (annual surveillance)

- In ~1996, Sandia entered the Stockpile Stewardship Program to develop comp-sim tools to (a) aid in decision making the absence/reduction of test data, and (b) improve the technical basis (i.e., understanding) of the basic physical processes that dictate weapon performance in all environments.

- As of ~2007, Sandia NW Engineering community is embracing comp. sim. (particularly high-fidelity comp. sim.) as an integral part of the NW design/analysis/qualification process.
  - Sandia NW Engineering is putting in place the policies, procedures, and peer reviews that essentially mandate V&V on all significant comp. sim. studies.

Sandia is Developing the Methods, Processes, Tools, and Training to Facilitate the Use of V&V/UQ

- **Methods Research Topics:**
  - **Verification:**
    - **Error estimation and finite element adaptivity for weapon applications**
    - **More complex analytic test problems that look like weapon applications**
  - **Validation:**
    - **Hierarchical validation of a system, with little/no system-level test data, based on test data and simulation data at subsystem and component levels**
    - **Bayesian calibration methods**
  - **Sensitivity Analysis / Uncertainty Quantification / QMU:**
    - **Adaptive sampling strategies for aleatory uncertainty propagation**
    - **Efficient epistemic+aleatory uncertainty propagation methods**
    - **Random field representation and propagation methods (intrusive and non-intrusive to codes)**
    - **Nonlinear sensitivity analysis methods**
    - **Parameter space dimensionality reduction methods**
- **Processes:**
  - **Software quality engineers now closely collaborating with code teams**
  - **Verification best practices documents for code teams**
  - **Validation best practices documents & training**
  - **Peer review using the <u>Predictive Capability Maturity Model</u>**

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Sandia is Developing the Methods, Processes, Tools, and Training to Facilitate the Use of V&V/UQ

- **Software Tools:**
  - Encore: mathematical methods for code verification
  - DAKOTA: math/statistics methods for optimization, sensitivity analysis, UQ
  - Validation software tools in works

- **Training / Education:**
  - Leverage existing in-house & external training, re: "Intro to Probability and Statistics," "Intro to Minitab Software," etc.
  - Leverage external V&V classes (e.g., Oberkampf & Roy AIAA V&V class)
  - ESP700 – Introduction to V&V/UQ
  - Encore & DAKOTA software user training
  - Attendance metrics: ~1600 attendees in ~40 training / education events since Aug 2007 (~800 unique attendees)
  - Streaming Video (Sandia internal): ~1200+ hits on V&V/UQ/QMU training video web site as of fall 2008

- **V&V/UQ/QMU info via Sandia Techweb:**
  - Search on "RMS" or "Records Management System", re: links to V&V/UQ reports, vugraphs, videos.
  - Go to Dept. 01544 web site, re: links to RMS + other V&V content.

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Key Issues:
(1) Most analysts do these activities formally/informally.
(2) Amount of formal V&V needed is driven by customer needs.

Overview of the Sandia V&V Process

PIRT Tables

1 DP Application

2 Planning

Understand the application and requirements

Assess capabilities, identify gaps, & prioritize work

Validation Experiment Centered Elements

4 Experiment Design, Execution & Analysis

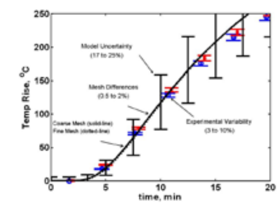
3 Code Verification

5 Metrics

3 Calculation Verification

6 Assessment

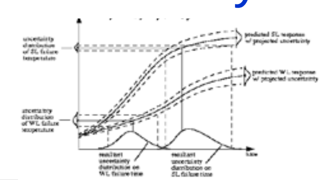
Compare to test data



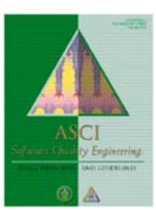
7 Prediction & Credibility

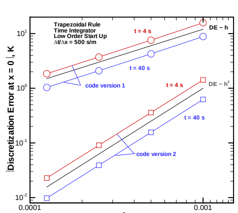
Document

Predictions w/ quantified uncertainty

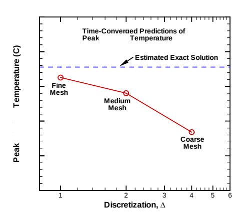


Software quality practices & numerical accuracy checks on test problems





Convergence checks on engineering application



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The Predictive Capability Maturity Model is our (Evolving) Approach to Answer: “How Good are the Codes?” and “Is that Sufficient?”

- **Intent of PCMM:**
  - Clarify the expectations of the customer, stakeholder, and project team with respect to rigor needed in a comp. sim. study.
  - Ensure that a consistent set of technical questions get asked of the team.
  - Illustrate progress, over time, across broad technical fronts.

- **PCMM is in Table Format (3 pages total):**
  - 7 main rows by 4 columns
  - Columns denote both “maturity level” of the technical work, and the “consequence level” of using the comp. sim. results in decision making:
    - 0 = low rigor / consequence
    - 1 = moderate rigor / consequence
    - 2 = high rigor / consequence; decisions informed via comp. sim. results
    - 3 = high rigor / consequence; decisions based primarily on comp. sim. results
  - Rows denote aspects of a comp. sim. study:
    - Geometric Fidelity [of the computer model vs. an as-built item]
    - Physics and Material Property Fidelity
    - Code Verification
    - Solution Verification
    - Validation
    - Uncertainty and Sensitivity Analysis
    - Documentation

Predictive Capability Maturity Model (PCMM)
Measures and Communicates Maturity of Mod/Sim Process

PREDICTIVIE ATTRIBUTE	Level 0 **Low-Consequence M&S-Informed, e.g., Scoping or Res Activities Score=0**	Level 1 **Low-Consequence M&S-Informed, e.g., Design Support Score=2**	Level 2 **High-Consequence M&S-Informed, e.g., Qualification Support, Score=4**	Level 3 **High-Consequence M&S-Based, e.g., Qualification Score=6**
Representation or Geometry Fidelity **Are you overlooking important effects because of defeaturing or stylization**	• Grossly defeatured or stylized representation based on judgment or practical considerations	• Significant defeaturing or stylization based on judgment or practical considerations • or lower fidelity representation justified w a significantly defeatured or stylized representation	• Limited defeaturing or stylization judged to retain the essential elements of "as built" • or appropriate lower fidelity representation justified w a slightly defeatured or stylized representation	• Highest fidelity representation "as is" w/o sig defeaturing or stylization • or appropriate lower fidelity representation justified w highest fidelity representation
Physics and Material Model Fidelity **How science-based are the models?**	• Unknown model form represented with ad hoc knob non-uniquely calibrated to IET • Empirical model applied w significant extrapolation, non-uniquely calibrated with IET	• Empirical model applied w/o significant extrapolation, uniquely calibrated with SET • Physics informed model applied w significant or unknown extrapolation, unique calibrations with SET • Physics-informed model applied w/o significant extrapolation, non-unique calibrations with IET	• Physics informed models applied w/o significant extrapolation, unique calibrations with SET • Physics-based model applied w significant or unknown extrapolation	• Well accepted physics-based model applied w/o significant extrapolation
Code Verification **Are software errors or algorithm deficiencies corrupting simulation results?**	• Judgment only	• Code managed to SQE standards • Sustained unit/regression testing w significant coverage of required Features and Capabilities (F&Cs)	• Code managed and assessed (internally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs	• Code managed and assessed (externally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs and their interactions
Solution Verification **Are numerical errors corrupting simulation results?**	• Judgment only • Sensitivity to discretization and algorithm parameters explored in SRQs not directly related to the decision context	• Sensitivity to discretization and algorithm parameters explored in SRQs directly related to the decision context • Numerical errors estimated in SRQs not directly related to decision context	• Numerical errors estimated in SRQs directly related to the decision context • Rigorous numerical error bounds quantified in SRQs not directly related to the decision context	• Rigorous numerical error bounds quantified in SRQs directly related to the decision context
Validation **How accurate are the models?**	• Judgment only • Qualitative accuracy w/o significant SET coverage	• Qualitative accuracy w significant SET coverage • Quantitative accuracy w/o assessment of unc and w/o significant SET coverage	• Quantitative accuracy w/o assessment of unc • w significant SET coverage and IETs	• Quantitative accuracy w assessment of unc • w significant SET coverage, IETs, and full system test
UQ and Sensitivities **What is the impact of variabilities and uncertainties on performance and margins?**	• 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	• 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	• Aleatory and/or epistemic uncertainties represented separately and propagated w/o significant strong assumptions • Quantitative sensitivity analysis w/o significant strong assumptions • Numerical errors quantified

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Predictive Capability Maturity Model (PCMM)
Measures and Communicates Maturity of Mod/Sim Process

PREDICTIVIE ATTRIBUTE	Level 0 Low-Consequence M&S-Informed, e.g., Scoping or Res Activities	Level 1 Low-Consequence M&S-Informed, e.g., Design Support	Level 2 High-Consequence M&S-Informed, e.g., Qualification Support,	Level 3 High-Consequence M&S-Based, e.g., Qualification
Representation or Geometry Fidelity Are you overlooking important effects because of defeaturing or stylization				
Physics and Material Model Fidelity How science-based are the models?				
Code Verification Are software errors or algorithm deficiencies corrupting simulation results?				
Solution Verification Are numerical errors corrupting simulation results?				
Validation How accurate are the models?				
UQ and Sensitivities What is the impact of variabilities and uncertainties on performance and margins?				

- **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).**

PCMM is Still Evolving:
e.g. PCMM (version 2) is now in use at Sandia

- **Status of PCMM within Sandia ASC:**
  - **PCMM self-assessments in use by ASC V&V project teams.**
  - **PCMM in use by some ASC V&V internal peer review panels.**
  - **ASC Program executives look for PCMM evidence for all Level-II milestones.**
    - **PCMM evidence now required for all ASC V&V-funded work.**

- **Other non-ASC programs at Sandia starting to investigate PCMM.**
  - **Nuclear weapons system engineering**
  - **DOD Work For Others projects using agent-based models**

PCMM Chart, Version 2 – Same General Structure, But Finer Granularity on Technical Practices (Rows)

PCMM Practice		Level 0	Level 1	Level 2	Level 3
Representation and Geometric Fidelity (RGF)	Characterization				
	Computation Error				
	Verification				
Physics and Material Model Fidelity (PMMF)	Science basis for models				
	Model Accuracy				
	Extrapolation				
	Technical review				
Code Verification (CVER)	Software Quality Engineering practices				
	Software Quality Assessment				
	Test coverage				
	Computation Errors				
Solution Verification (SVER)	Numerical Solution Errors				
	Input/Output Verification				
	Technical Review				
Validation (VAL)	Validation hierarchy				
	Model Accuracy				
	Extrapolation				
	Technical review				
Uncertainty Quantification (UQ)	Uncertainty Characterization and Interpretation				
	Sensitivity Analysis				
	Numerical Propagation Errors				
	Aggregation of Evidence for Characterization of Uncertainties				
	Completeness				
	Strong Assumptions				
	Technical Review				
Documentation and Archiving	Documentation and Archiving				

Outline

- Introduction
- Background on:
  - Verification & Validation (V&V)
  - Quantification of Margins and Uncertainties (QMU)
- Engineering Application
- V&V at Sandia Today
- Predictive Capability Maturity Model (PCMM)
- **Summary**

Summary

- Sandia's science & engineering practices are evolving to include V&V, UQ, and QMU methods.
  - Enable risk-informed decision making on high-consequence applications.
    - Use sensitivity/UQ methods to get better, more complete answers
    - Employ V&V as an "evidence" tool for comp. sim.
- Science front:
  - Research, develop, and deploy new mathematical and statistical methods that improve V&V practices.
  - Leverage validation results to identify physics research topics.
- Engineering front:
  - Establish integrated teams: engineers, scientists, math/stats, etc.
  - Provide tools and training to facilitate use of V&V/UQ methods.
  - Select appropriate level/depth of V&V/QMU effort for each weapon application (via customer-desired PCMM "maturity" level).
  - Use V&V/UQ methods to deliver "best estimate + quantified uncertainty and margins" to customers.

References: Sandia V&V/UQ/QMU Publications & Related Items

PCMM

W. L. Oberkampf, M. Pilch, and T. G. Trucano, "Predictive Capability Maturity Model for Computational Modeling and Simulation," Sandia Report SAND2007-5948, Sandia National Laboratories, Albuquerque, NM, 2007.

QMU

T. Trucano, M. Pilch, and J. Helton, "Ideas Underlying Quantification of Margins and Uncertainties (QMU): A White Paper," Sandia Report SAND2006-5001, 2006.

K. V. Diegert, S. E. Klenke, G. C. Novotny, R. A. Paulsen, Jr., M. Pilch, T. G. Trucano, "Toward a More Rigorous Application of Margins and Uncertainties Within the Nuclear Weapons Life Cycle: A Sandia Perspective" Sandia Report SAND2007-6219, Sandia National Laboratories, Albuquerque, NM, 2007.

(NEW) J. C. Helton, "Conceptual and Computational Basis for the Quantification of Margins and Uncertainty," Sandia Report SAND2009-3055, Sandia National Laboratories, Albuquerque, NM, 2009.

2008 National Academy of Sciences QMU review: "Evaluation of Quantification of Margins and Uncertainties Methodology for Assessing and Certifying the Reliability of the Nuclear Stockpile" (http://www.nap.edu/catalog.php?record_id=12531)

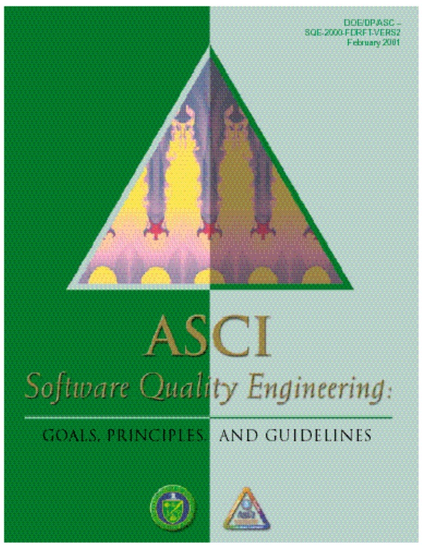
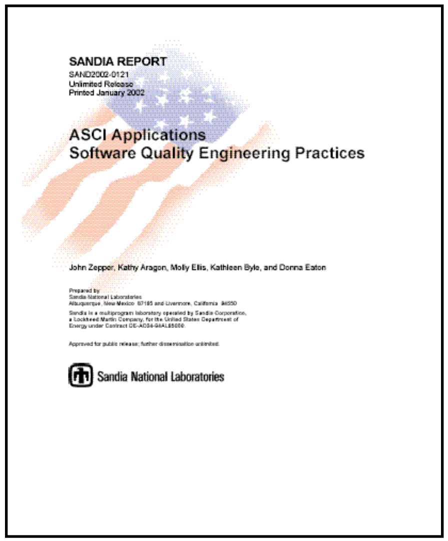
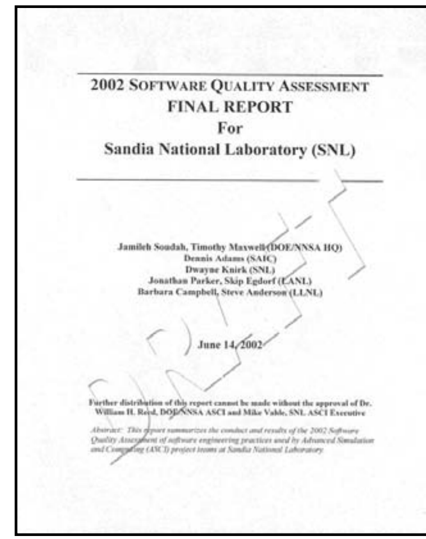
Extra / Backup Slides

Example Engineering Application: Aircraft Crash and Weapon in a Fire

- What types of performance measures is the computational simulation capability expected to predict?
  - System performance measures:
    - Ex: Maximum temperature
  - Reliability performance measures:
    - Ex: Mean time to failure
  - Safety performance measures:
    - Ex: Probabilities on safety margins
- What is the accuracy required for each performance measure?

Mock Aircraft Wing and Fuselage

Software Quality Engineering: Requirements and Assessments

Tri-Lab Guidelines	Lab-Specific Requirements	Indep. Internal Assessment	Indep. External Assessment
			

SNL/ASC Quality Management Council (AQMC)

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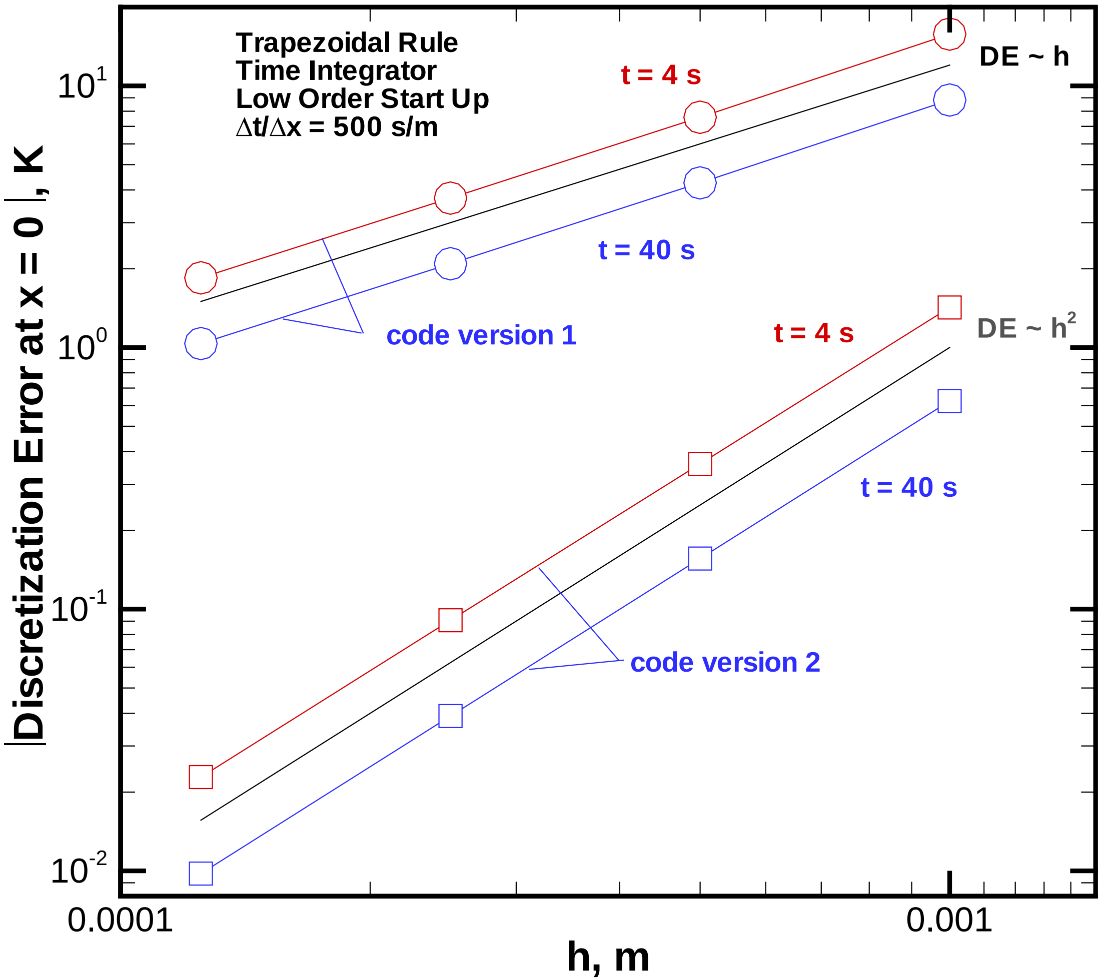
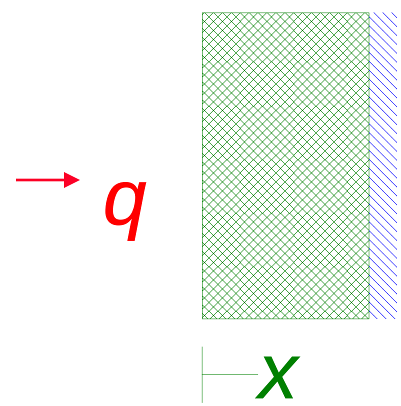
Code Verification Example: Demonstrating the Correct Rate of Spatial Convergence on Analytic Tests



- VERTS mapped to required physics and code capabilities
- Code Verification of Calore (thermal response code) found bugs
- Code bug discovered and fixed based on priority and resource availability. Status tracked in code issue log, which can be accessed by analysts

- Transient response of planar 1-D slab to constant flux



Modeled as full 3-D object

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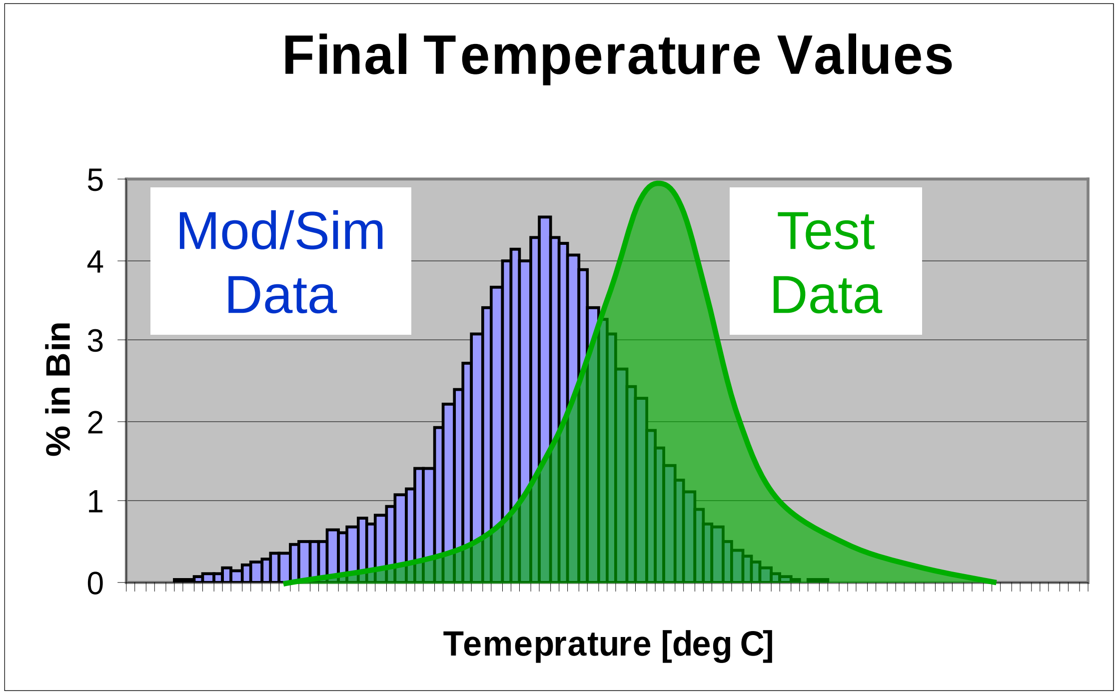
Example of Uncertainty Quantification and Validation



Uncertainty Quantification:
- UQ methods generate ensemble of mod/sim data.

Validation:
- Compare simulation data histogram to a test data histogram.
  - Quantify amount of "overlap" between histograms.
  - Assess sufficiency of overlap.

- **UQ methods provide statistical info on the code output data:**
  - **Probability distribution on Temperature, *given various $x_1,...,x_N$ inputs.***
  - **Correlations (trends) of Temperature vs. $x_1,...,x_N$.**
  - **Mean(T), StdDev(T), Probability($T > T_{critical}$)**

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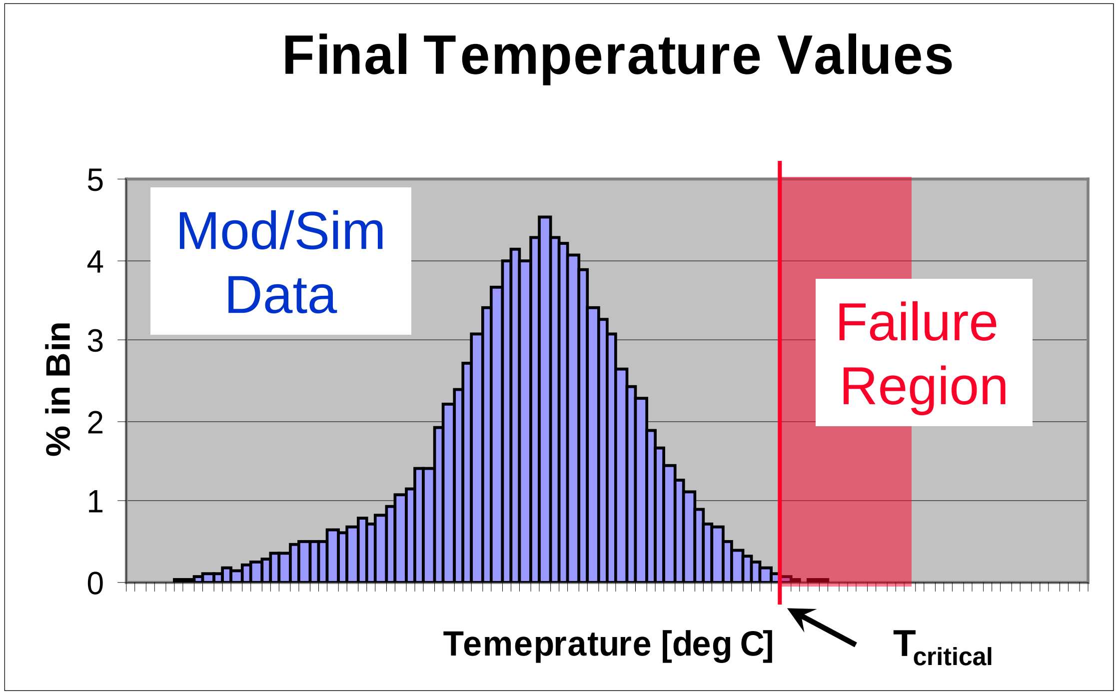
Example of Uncertainty Quantification and QMU



Uncertainty Quantification:
- UQ methods generate ensemble of mod/sim data.

Quantified Margins & Uncertainties:
- Estimate failure probability.
- Compare *estimated* failure probability to *allowable* failure probability, including all sources of uncertainty.

- **UQ methods provide statistical info on the code output data:**
  - **Probability distribution on Temperature, *given various $x_1,\ldots,x_N$ inputs.***
  - **Correlations (trends) of Temperature vs. $x_1,\ldots,x_N$.**
  - **Mean(T), StdDev(T), Probability($T > T_{critical}$)**

Close-up View of Validation Plot