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 <u>shall incorporate QMU methodologies</u> 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 <u>Quantification of Margins and Uncertainties</u>."**

- **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.**

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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)**

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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)**

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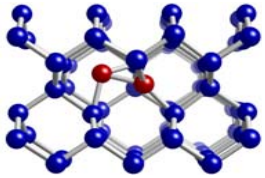
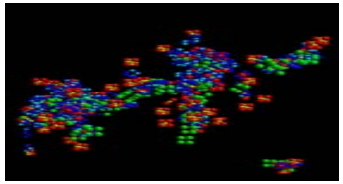
V&V/UQ/QMU Thinking is Embedded in Sandia's QASPR Project

- **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.**

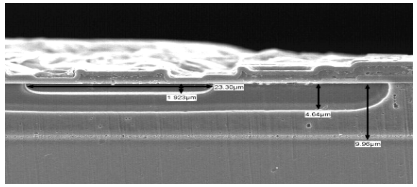
Radiation Env: x-rays, gamma rays, neutrons, etc.

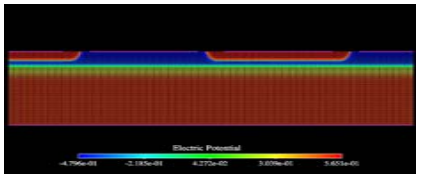
Atomic-scale defects



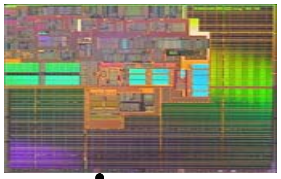


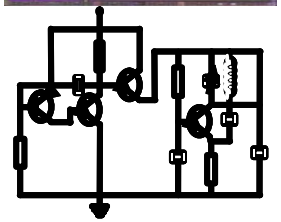
Device effects (transistor, diode, etc.)



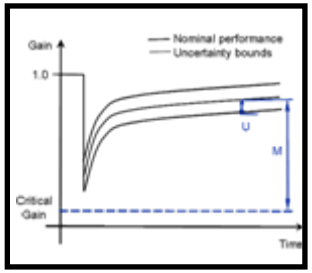


Circuit effects





QMU Assessment



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

1 DP Application

Understand the application and requirements

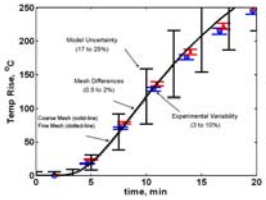
2 Planning

Assess capabilities, identify gaps, & prioritize work

4 Experiment Design, Execution & Analysis

Validation Experiment Centered Elements

Compare to test data



3 Code Verification

5 Metrics

3 Calculation Verification

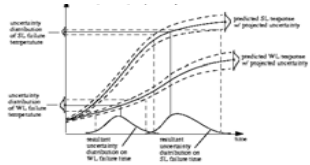
6 Assessment

Software quality practices & numerical accuracy checks on test problems

Convergence checks on engineering application

Predictions w/ quantified uncertainty

7 Prediction & Credibility



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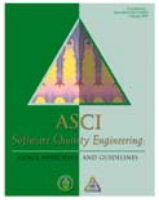

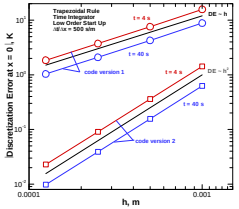

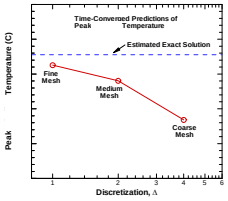

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What's New in Sandia's V&V/UQ/QMU?

- **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 <u>assess and communicate</u> evidence supporting credibility of simulations.**

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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 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				
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?			• Sensitivity to numerical errors explored	• Numerical errors quantified

- **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).**

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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.**

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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.**

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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.**

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Points of Contact

- **Tony Giunta's contact info:**
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  - **Email: aagiunt@sandia.gov**

Backup Slides

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 <u>assess and communicate</u> evidence supporting credibility of simulations.**
  - **Stress <u>practical</u> VV-UQ-QMU, <u>training</u>, and <u>teaming</u>**

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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 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).**

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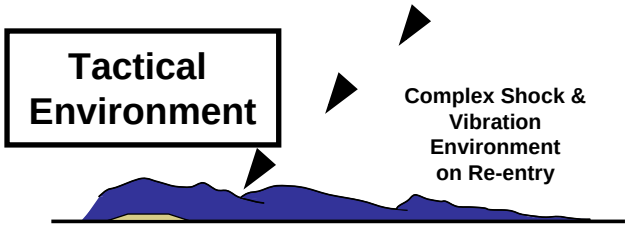
Typical QMU Application

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”.

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Predictive Capability Maturity Model: Example Self-Assessment (Goal is Level 2)

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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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 <u>all</u> projects, and, will be reviewed by managers/peers.**
  - **Continued emphasis on practical VV/UQ/QMU approaches.**

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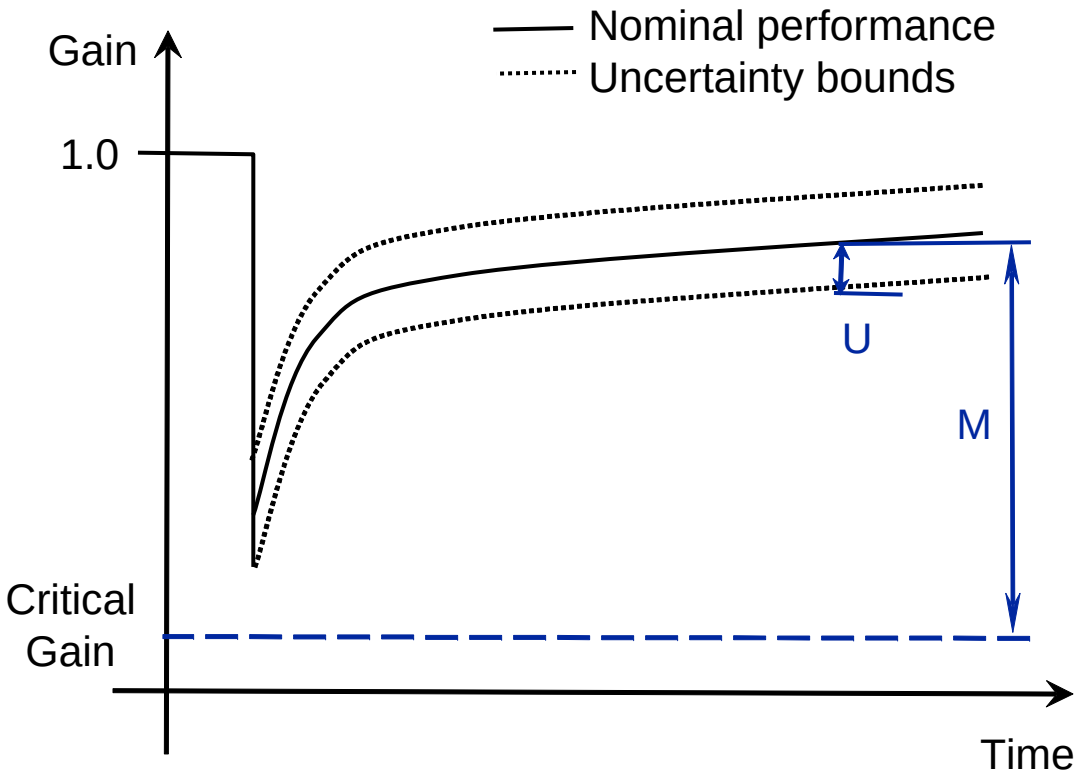
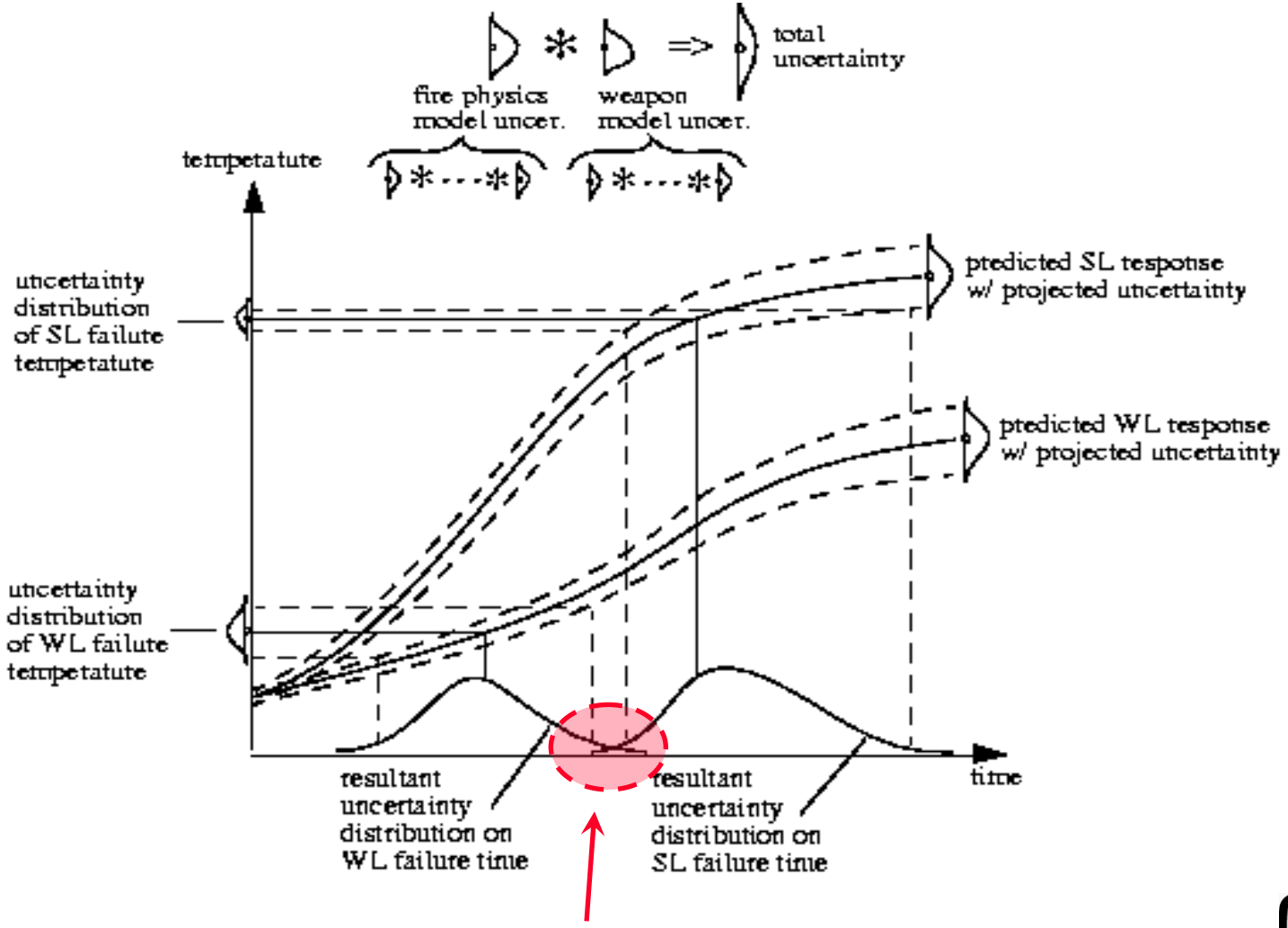
Predictions w/ Quantified Uncertainty

- **QMU: Use simulations, and quantified uncertainties, for performance predictions and margin estimates at <u>untested</u> conditions. – *via DAKOTA***
  - **And, <u>assess adequacy</u> 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.