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Title:

ENGINEERING APPLICATIONS OF LARGE-SCALE COMPUTING: DISCUSSION OF THE CHALLENGES AND OPPORTUNITIES OF TERAOPS COMPUTING (U)

Author(s):

François M. Hemez, Los Alamos National Laboratory, ESA-WR

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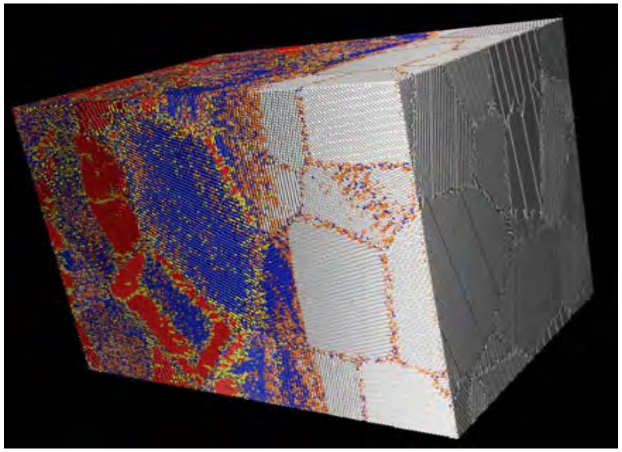
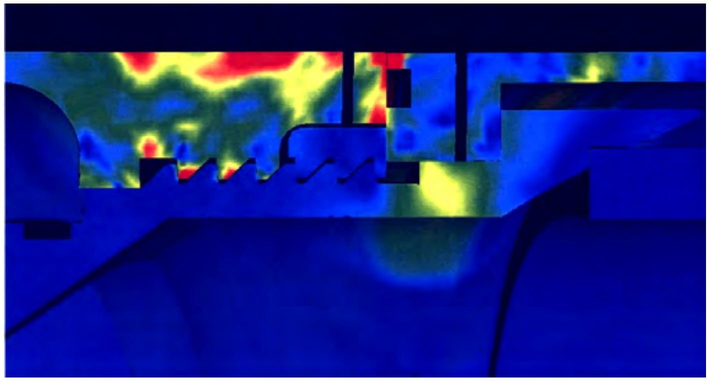
ENGINEERING APPLICATIONS OF LARGE-SCALE COMPUTING (U)





François M. Hemez

Los Alamos National Laboratory
Engineering Sciences and Applications
ESA-WR, Mail Stop T006
Los Alamos, New Mexico 87545
hemez@lanl.gov

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Abstract

Current computing resources make it possible to model and analyze increasingly complex physical phenomena. One such example is the Department of Energy's ASCI (Accelerated Strategic Computing) program. The ASCI program is developing platforms capable of 10^{+13} multiplications per second (over 10 TeraOps) by distributing the computations among thousands of processors. Large resources are also devoted to the development of multi-physics, multi-scale analysis codes and the validation of numerical models. Examples of problems that require access to such resources are the global climate prediction, computational genetics, molecular dynamics and thermonuclear physics.

The TeraOps approach to solving complex problems is becoming increasingly popular. Japan has built a 35 TeraOps computer to study the global seismic activity and the United Kingdom has recently bought 5 platforms each capable of 5+ TeraOps. When applied to engineering problems, it is discovered that, instead of replacing prototyping and testing, TeraOps computing rather promotes a change in the nature of testing. Physical experiments are changing from qualification tests to validation experiments. The objective of a validation experiment is, for example, to validate the physical laws implemented in an analysis code and determine the operational space within which a model can be implemented with confidence.

This presentation offers an overview of challenges and opportunity of TeraOps computing. Our perspective is that of users, not code developers nor computer scientists. Needs in terms of uncertainty quantification and model validation are emphasized. Some of the techniques recently applied to various problems include the design of experiments, non-probabilistic theories for representing uncertainty and global sensitivity analysis. Several engineering applications are used as examples to illustrate the discussion.

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The Relationship Between Experiments and Simulations is Changing …

- **Old paradigm: Experiments are qualification tests, proof that something does or does not "break". Simulations are used to understand the behavior (generally, after the fact).**

- **New paradigm: Experiments explore the mechanics and validate predictions. Simulations are used to predict, with *quantifiable confidence* and across the *operational space*.**

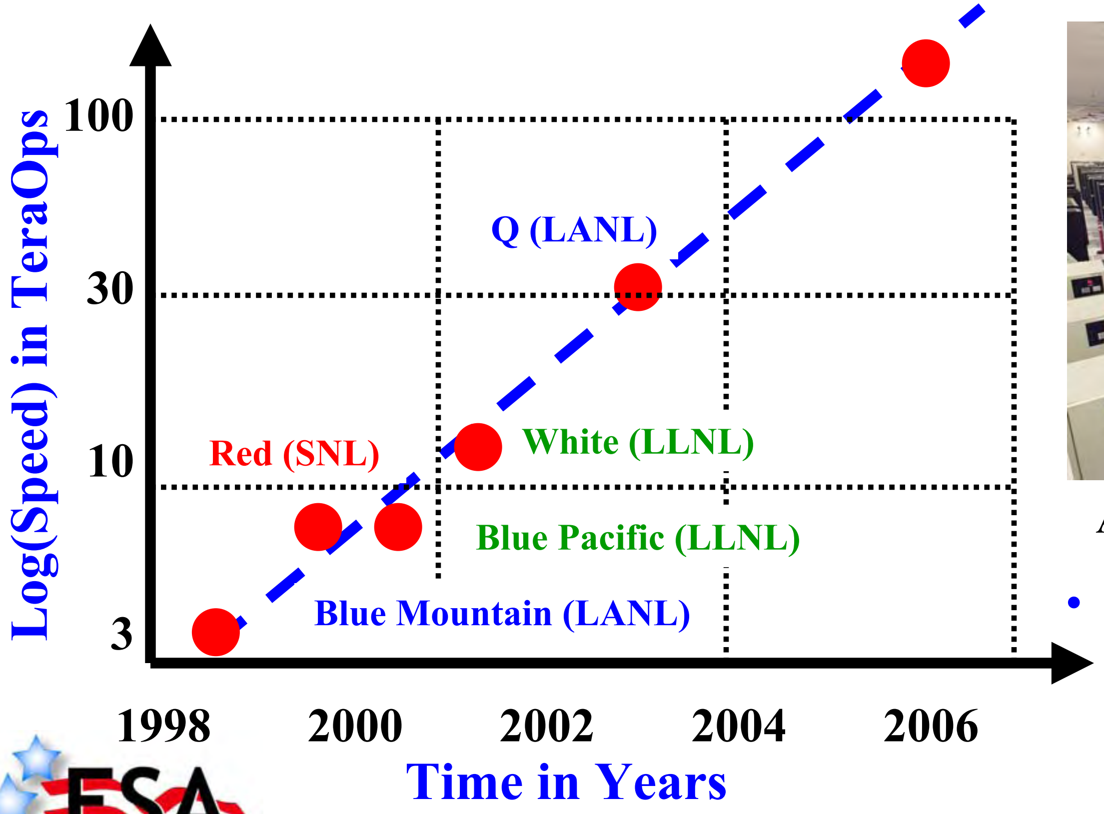
- **Objective: Make decisions based on the predictions from *validated* science-based simulations. "Validation" requires an assessment of the sources of uncertainty (including the *lack-of-knowledge*) and their effects on the decision.**

What is Driving Such Radical Change?

- In many industries a competitive advantage is sought by reducing the time it takes to design, test, and field a new product.
- To lower production costs, design conservatism must be reduced without increasing the budget allocated to testing.
- U.S. National Laboratories are being asked to "certify" the nuclear weapon stockpile without full-scale testing.
- Generally accepted belief that predictive accuracy can be reached if enough "details" are included in the models.

Extreme Computing

- **ASCI platforms at Los Alamos (LANL), Livermore (LLNL), and Sandia (SNL) National Laboratories deliver TeraOps (1 TeraOps = 10^{+12} FLOPS) capabilities:**



ASCI Q at Los Alamos (Nov. 2002)

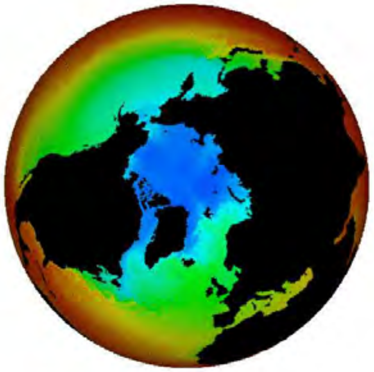
- **ASCI platforms make it possible to analyze high-fidelity models *and* perform more runs.**

Science-based Simulation

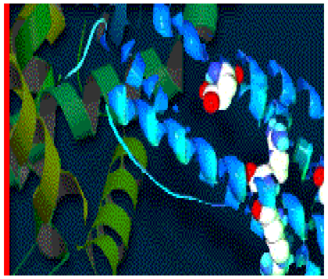
- Developing theories and modeling Nature are 4,000+ years old scientific activities. Science-based prediction is a new endeavor (20+ years old).
- Current trends are the high-fidelity description of the geometry; inclusion of more coupled physics; modeling of multiple-scale phenomena.
- Science-based prediction's Achilles heel is *credibility*, or accumulating evidence of the predictive accuracy of numerical simulations.

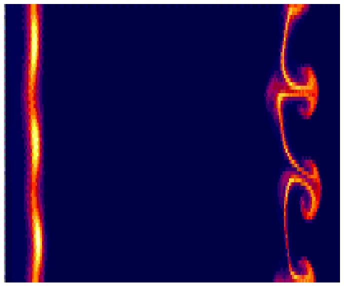
From the Trojan war: Achilles fighting Penthesilea, (Athens, Greece, 530 BC).

Examples of Really Difficult Problems

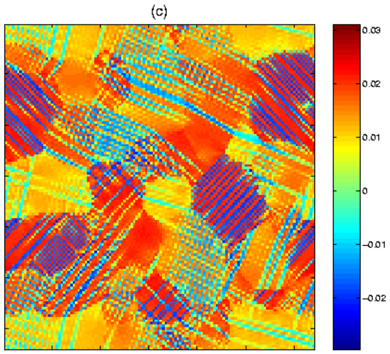


- Global climate modeling.
- Protein folding.



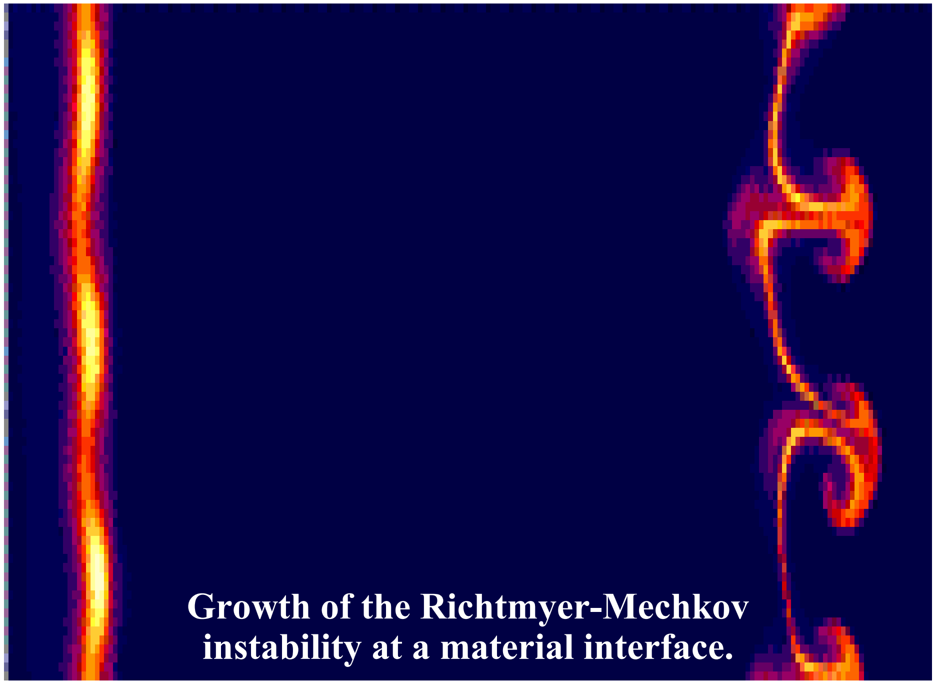


- Richmeyer-Meshkov instabilities.
- Understanding the properties of metals from the grain size (or molecular size) and up.



What Does it Take to Certify Our Systems?

- System certification requires *unprecedented physics-based simulations* because testing cannot be performed.
  - First full-system, full-physics, 3D simulations of a nuclear weapon detonation completed in March 2002.
  - Required 7 months (5,040 hours) of the 6,000+ processors of Blue Mountain, a 3 TeraOps ASCI platform at Los Alamos.
  - The number of equivalent single CPU hours is 3,584 years!

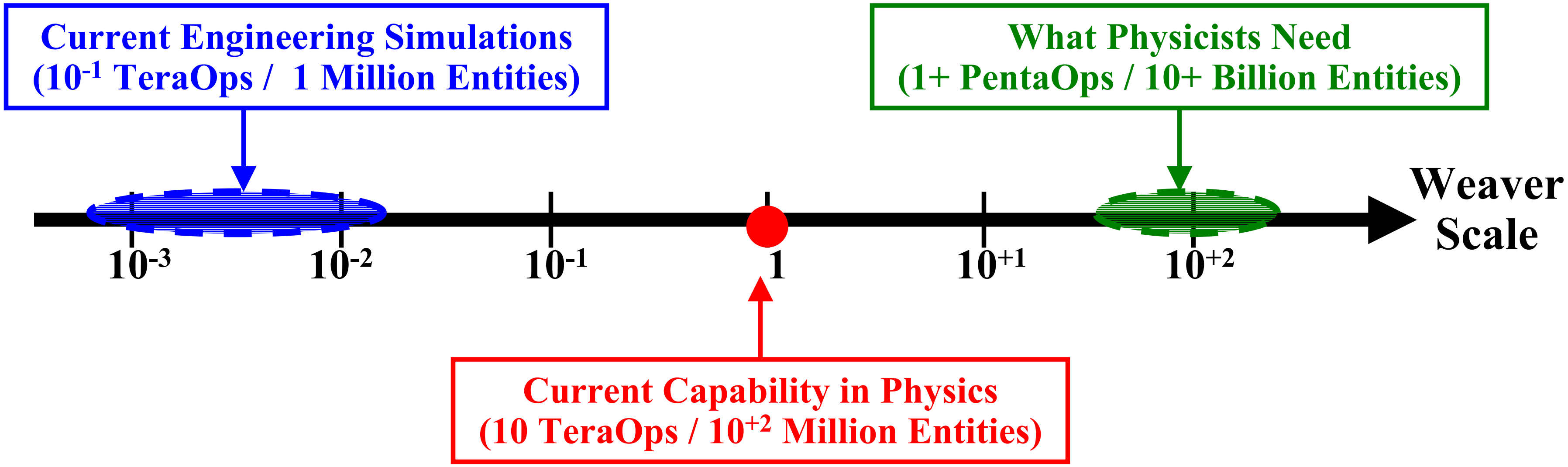


Growth of the Richtmyer-Mechkov instability at a material interface.

- Is there more to these numbers than pretty pictures?

High-level Overview of Our Needs in Terms of Computational Resources …

- Our "Weaver" scale† provides a qualitative description of computational capabilities and needs. (†Named after Bob Weaver, X-2.)



Current Engineering Simulations
(10^{-1} TeraOps / 1 Million Entities)

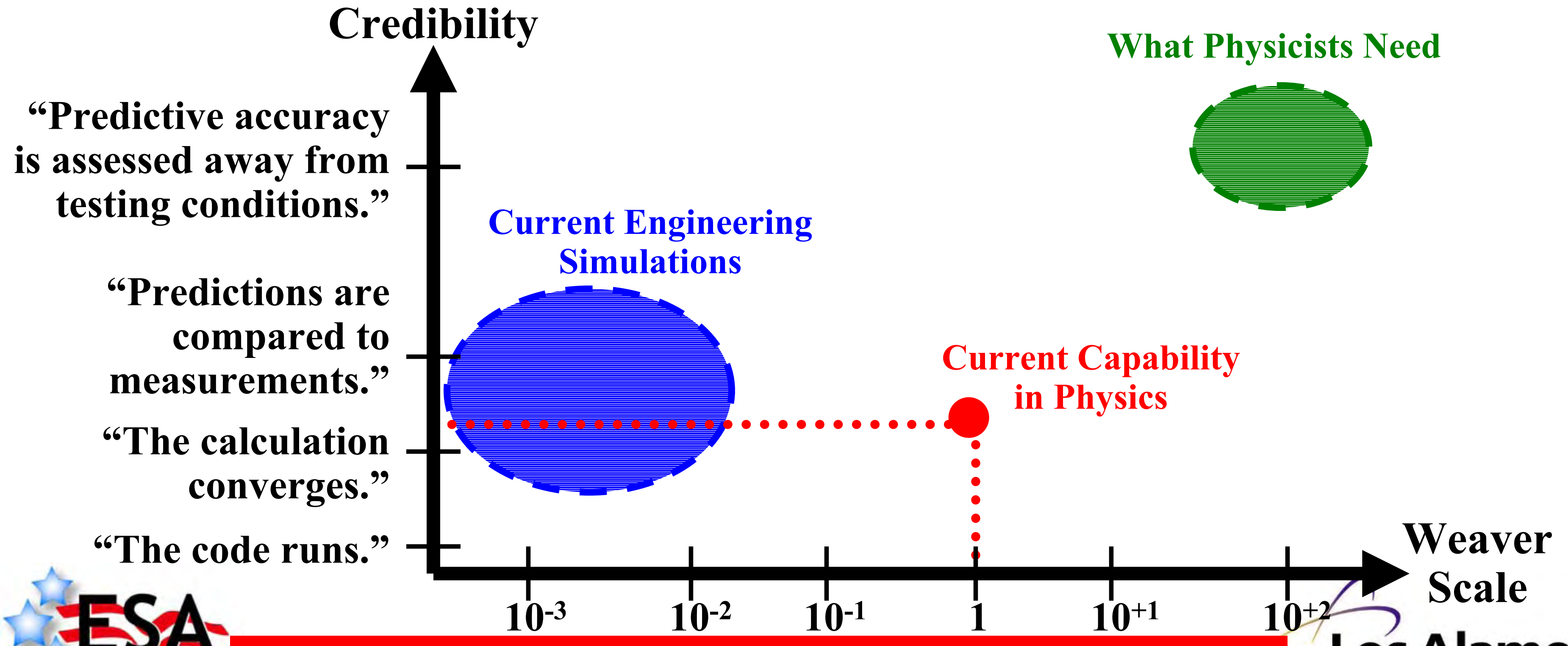
What Physicists Need
(1+ PentaOps / 10+ Billion Entities)

Current Capability in Physics
(10 TeraOps / 10^{+2} Million Entities)

Note 1: Scale always centered about current capability in physics.
Note 2: 1 TeraOps = 10^{+12} FLOPS; 1 PentaOps = 10^{+15} FLOPS.

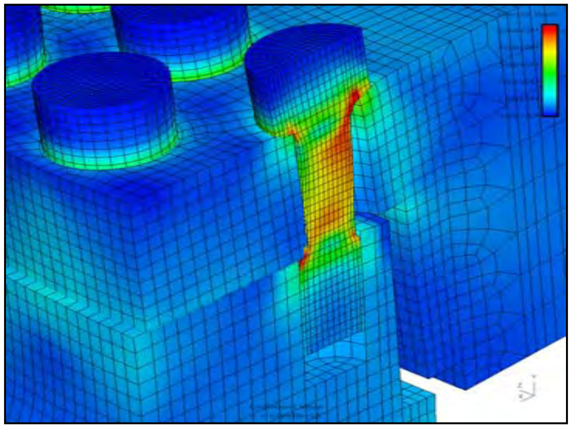
High-level Overview of Our Needs in Terms of Prediction Credibility …

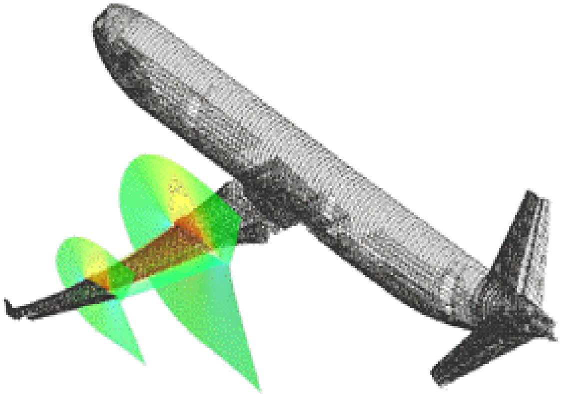
- **The ability to assess prediction *credibility* is currently 1+ order of magnitude less than what is needed … because of the challenges offered by the quantification of *uncertainty*.**



Engineering Applications

- TeraOps computing lets us analyze complex systems with an unprecedented level of detail and accuracy.
- TeraOps computing can make some of our modeling rules become obsolete.
- TeraOps computing can help us discover new phenomena.

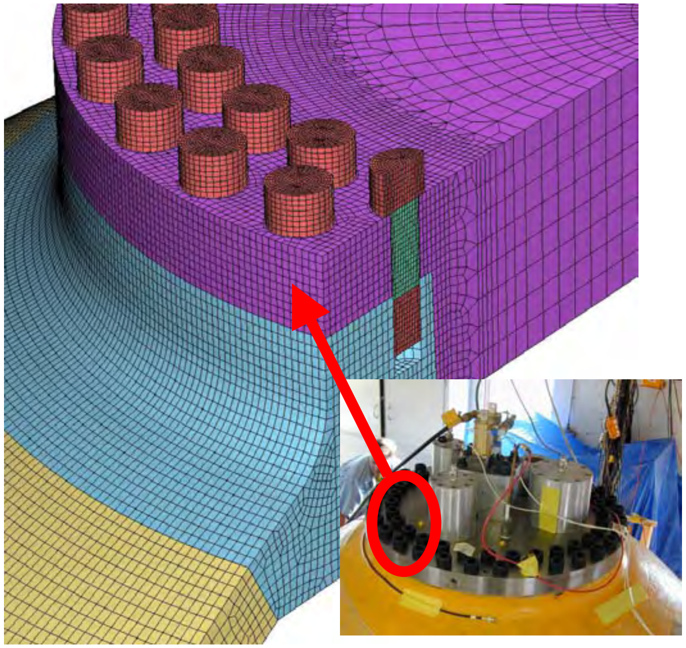




Qualification of Containment Vessels

- **Pre-testing qualification of explosive containment vessels for the radiography of hydrodynamic experiments.**
- **Need to assess the risk to accidentally release contaminant material *prior* to performing the experiments.**

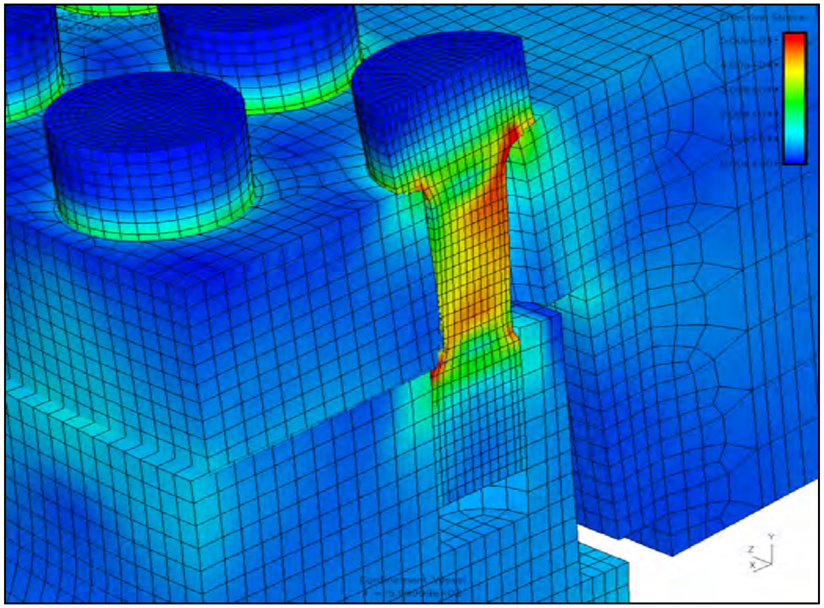
Containment Vessel



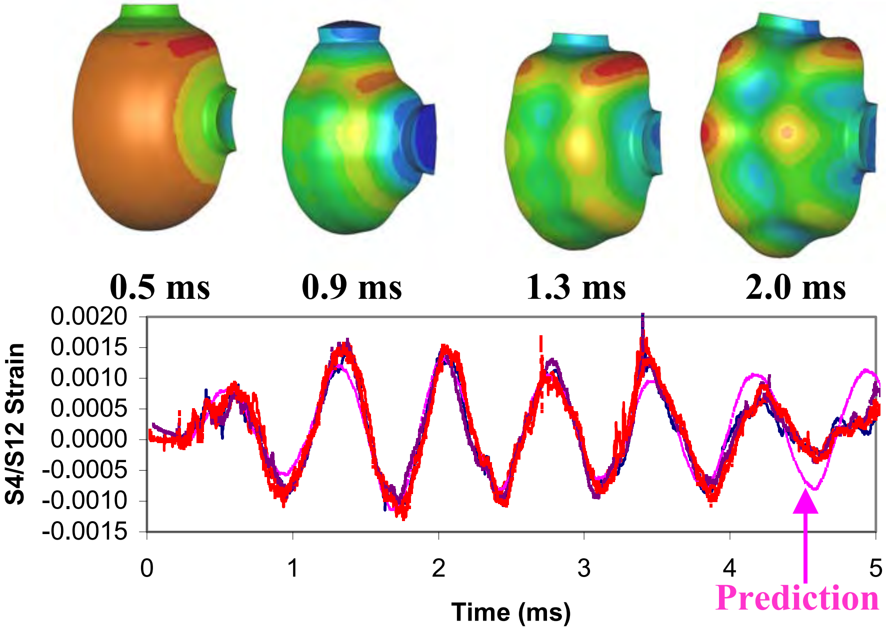
Detail of the Computational Mesh

Qualification of Containment Vessels

- High-fidelity models (10 Million unknowns, full contact) are analyzed to evaluate the risk of material leakage.



Simulation of a Potential Leak Path



Comparison of Measurements and Predictions

- The measurements collected during the tests demonstrate excellent predictive accuracy.

High-fidelity Modeling of HE

- **The prediction accuracy of an unprecedented constitutive model of High Explosives (HE) is quantified.**

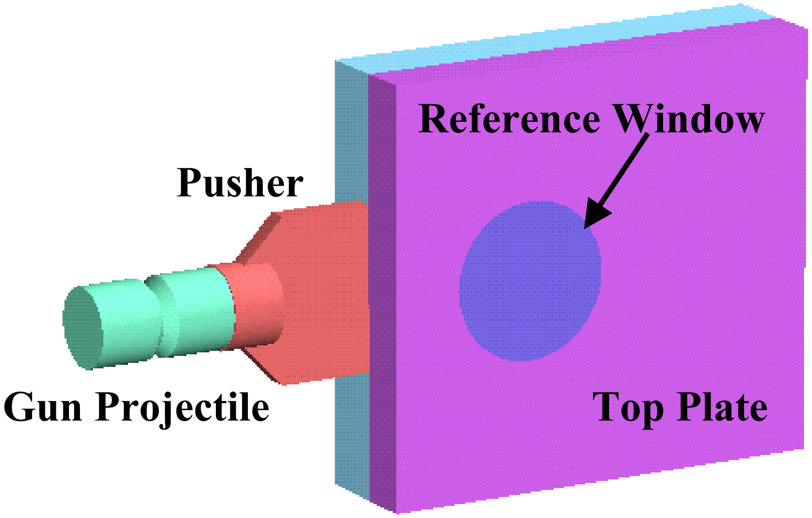
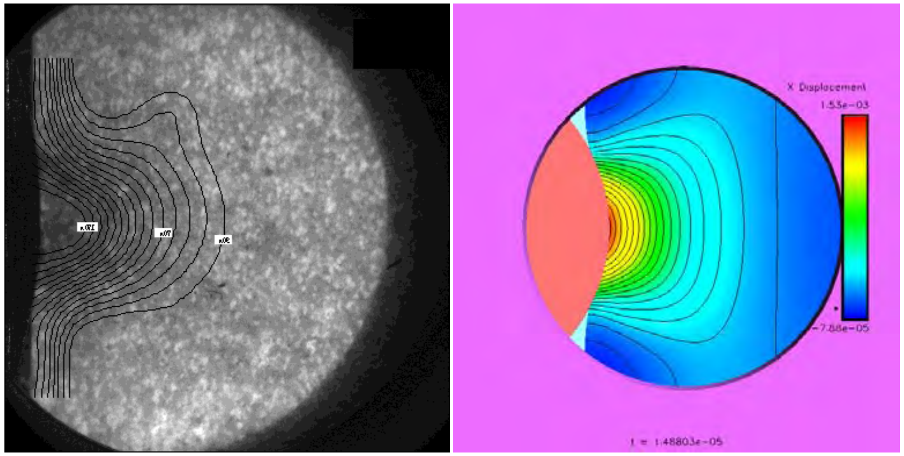


Illustration of an Impact Experiment



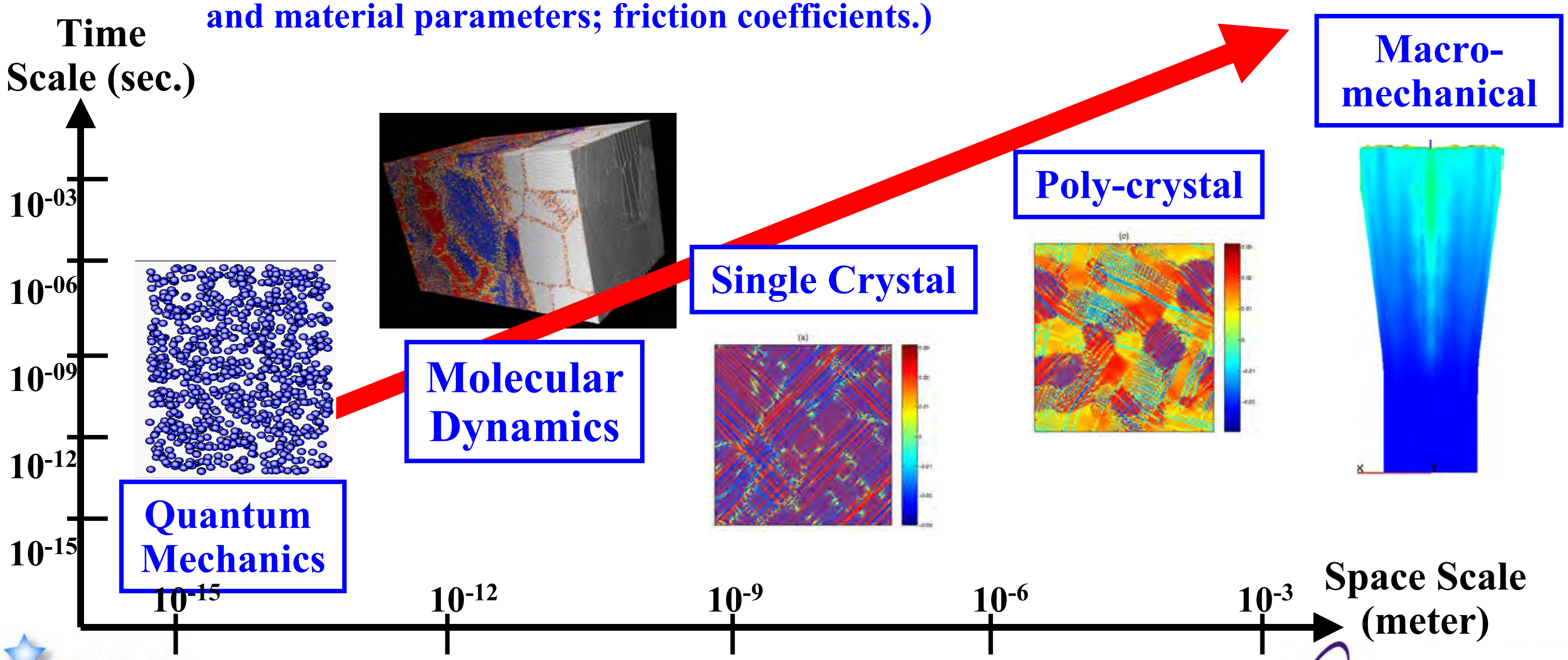
Validation of the Visco-SCRAM Model

- **The Visco-SCRAM model includes strain-rate dependent mechanics, fracture behavior, thermal properties, and ignition criteria.**

First-principles Physics

- Some of the information needed to define high-fidelity models must be obtained from "first-principles" physics.

(Examples: parameters of the shock-physics models; equation-of-state and material parameters; friction coefficients.)



Quantum Mechanics

Molecular Dynamics

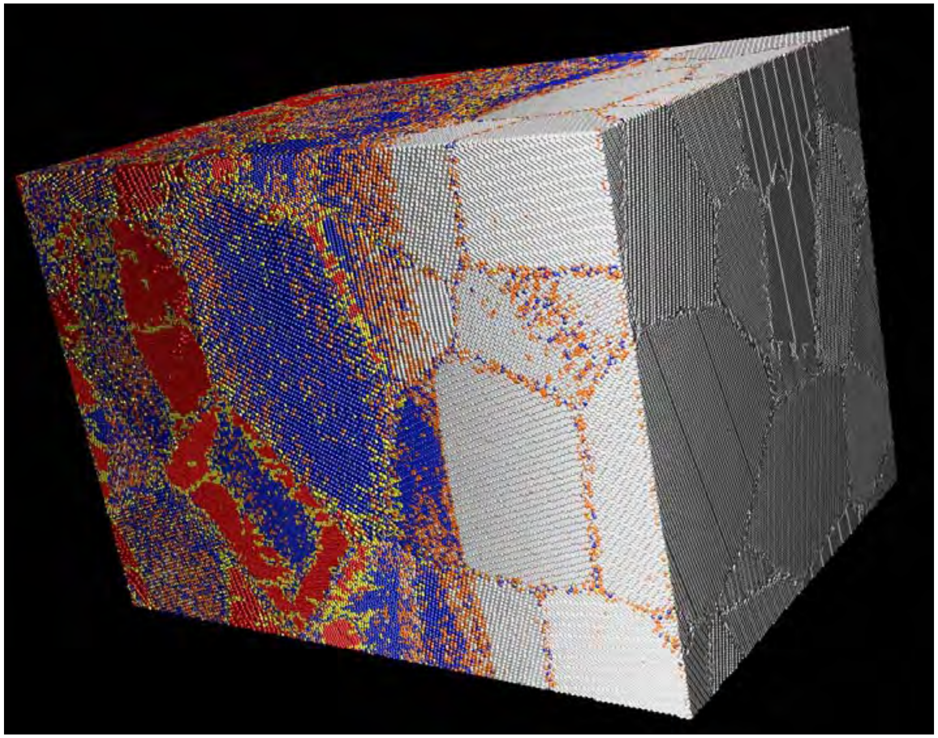
Single Crystal

Poly-crystal

Macro-mechanical

Shock Physics at the Atomistic Scale

- Molecular dynamics are used to study shock propagation and aspects of phase transformation at the atomistic level; guide parameters and physics of single-crystal modeling.

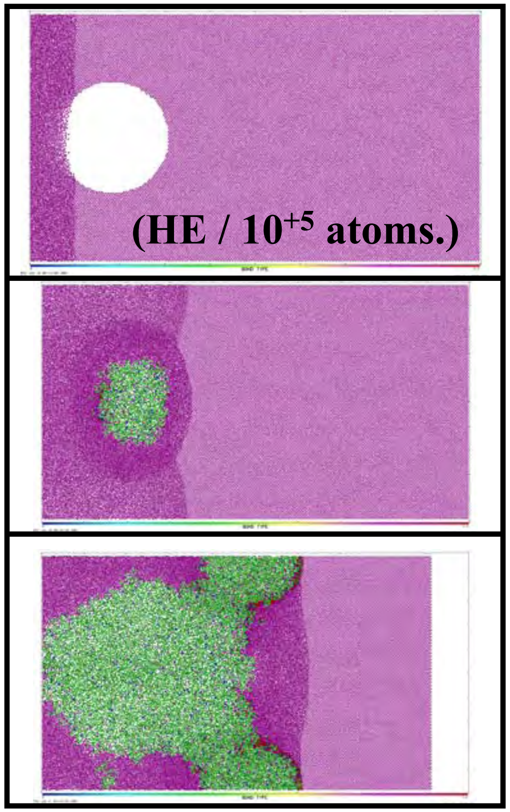


  - Propagation of a shock wave through a material that exhibits a grain structure.
  - Simulation performed with a parallel code and 100 Million particles (10^{+8} particles).
  - Time scale: 10 pico-second (10^{-11} second).
  - Length scale: 1 nanometer (10^{-9} meter).

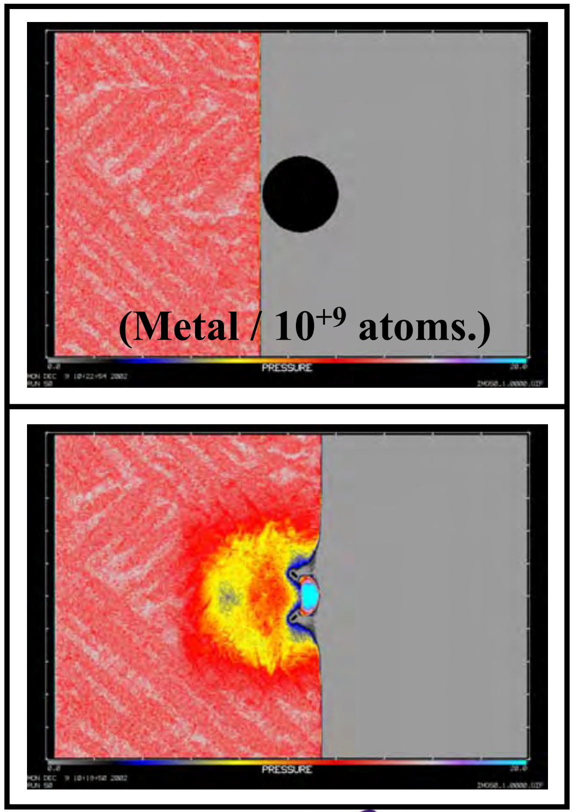
(Credit: T-11, T-12, X-7 at LANL.)

Void Collapse at the Atomistic Scale

- Molecular dynamics simulations guide the development of continuum models of 2D void collapse in materials.
  - Chemical reactions can be produced when a shock travels through the material.
  - The initial shock does not cause reaction.
  - The void collapse boosts the shock pressure.
  - Interaction of waves leads to detonation.



(Credit: T-14, MST-8 at LANL.)



(Credit: T-11, T-12, X-7 at LANL.)

A Quick Summary of What We Have Established So Far …

- Need to qualify systems without full-scale testing. Science-based prediction is the only alternative to lack of testing.

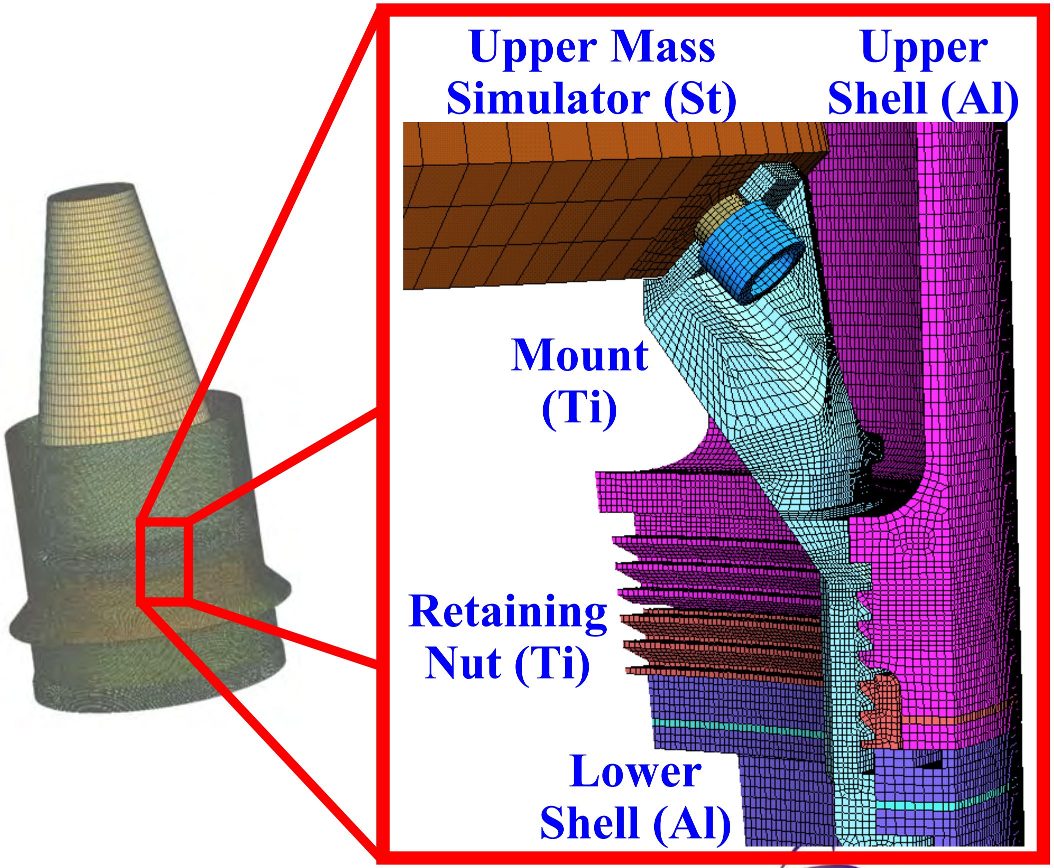
- Prediction accuracy can be achieved through combination of Tera-scale computing and high-fidelity modeling.

- First-principles physics can provide critical insight and estimation of scaled-up model parameters.

- To demonstrate credibility (i.e., provide confidence), the sources of uncertainty and their effects must be assessed. *Uncertainty quantification* is arguably the most important component of prediction accuracy assessment.

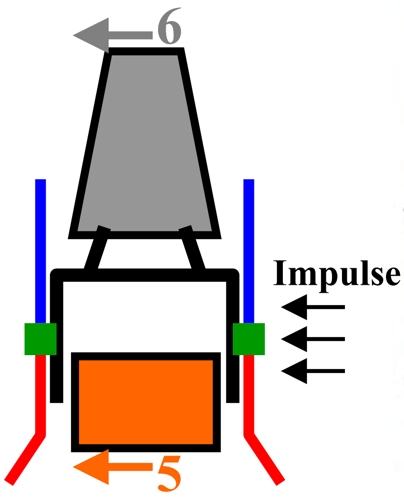
Qualifying Engineering Systems Requires to Understand the Sources of Uncertainty …

- Assembly of components held together by a large thread:

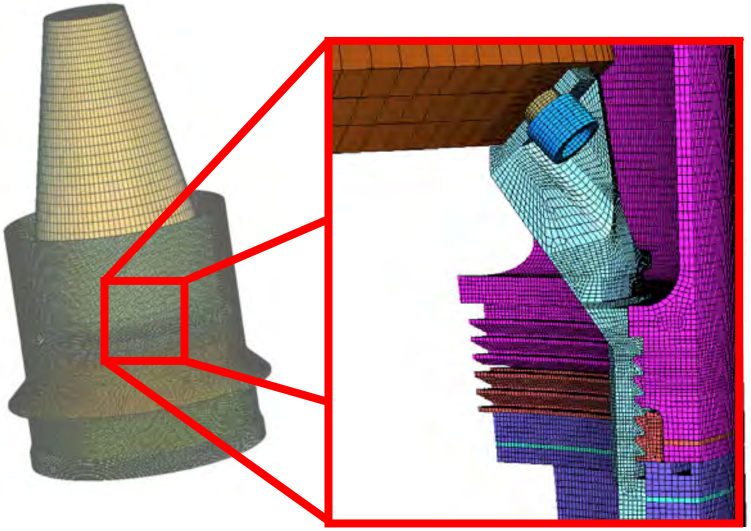


Modeling of the Threaded Assy.

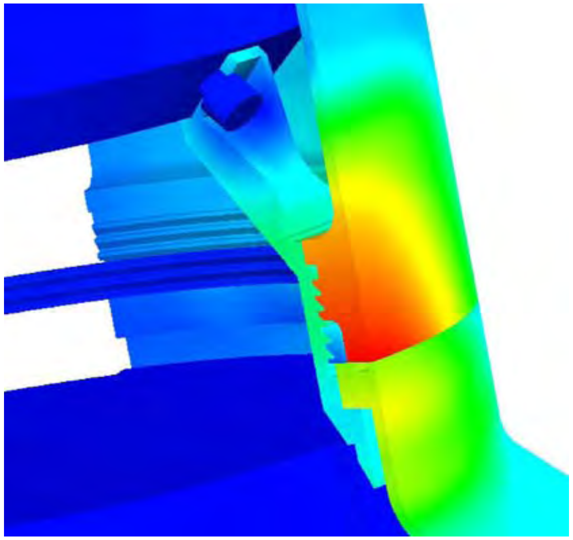
- **The LLNL/ParaDyn explicit simulation currently counts over 1.4 Million elements, 480 contact pairs, and 6 Million degrees-of-freedom.**



Sensors 5 & 6



Detail of the Computational Mesh

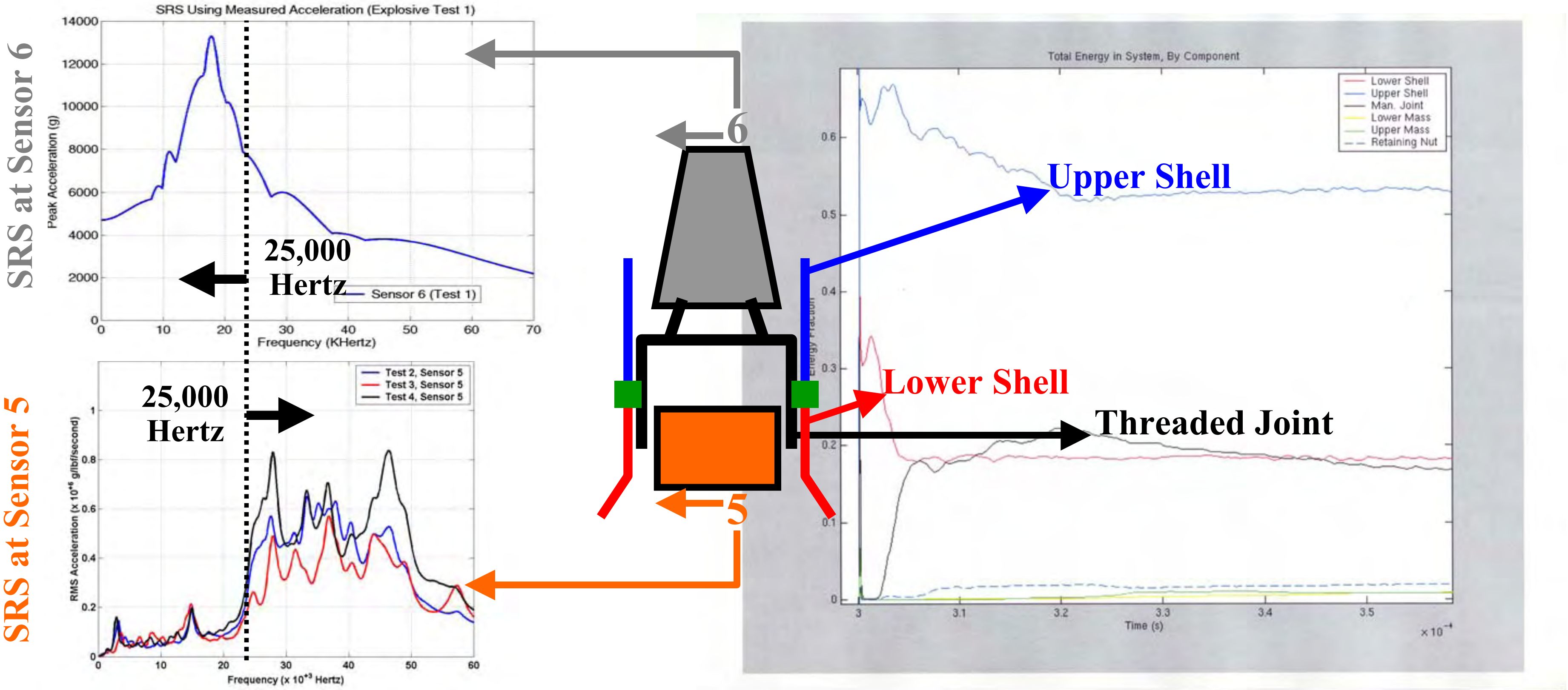


Displacement Contour

- **Each run requires 4 to 5 hours to simulate 3 milliseconds of response using 504 processors of ASCI Blue Mountain.**

Energy Flow

- **The threaded mount prevents energy from flowing to the critical payloads, “filters” the shock frequency spectrum.**

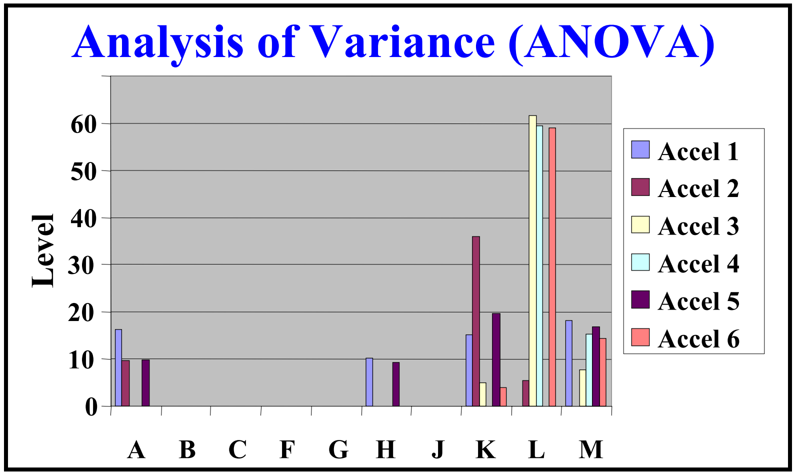


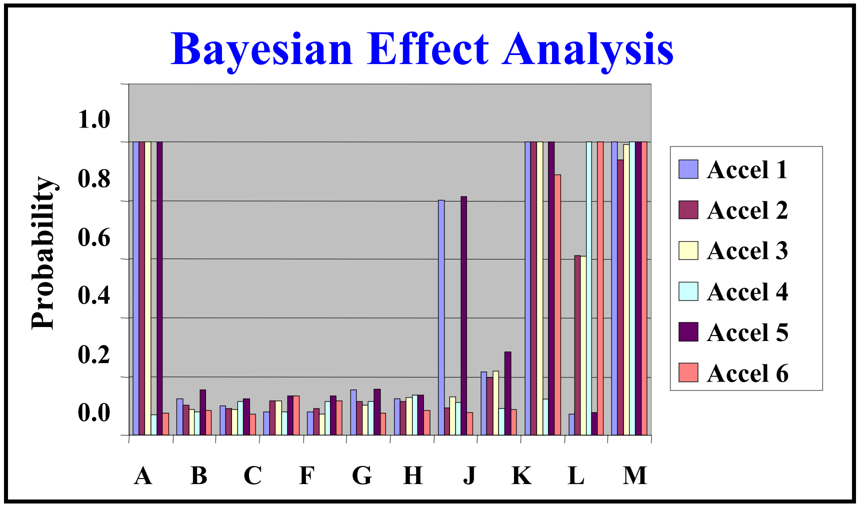
From Test Data

From Numerical Simulations

Effect Screening

- Design of (computer) experiments, effect screening, and meta-modeling are used extensively to manage variability and randomness.


Analysis of Variance (ANOVA)


Bayesian Effect Analysis

12 Random Variables of the Threaded Assembly Simulation

Preloads:	Static friction:	Kinetic friction:	Input Loading:
• A, Tape joint	~~• D, Al/Al static~~	~~• H, Al/Al kinetic~~	• M, Impulse level
~~• B, Retaining nut~~	~~• E, Ti/Ti static~~	• J, Ti/Ti kinetic	
~~• C, Upper shell~~	~~• F, Al/Ti static~~	• K, Al/Ti kinetic	
	~~• G, St/Ti static~~	• L, St/Ti kinetic	

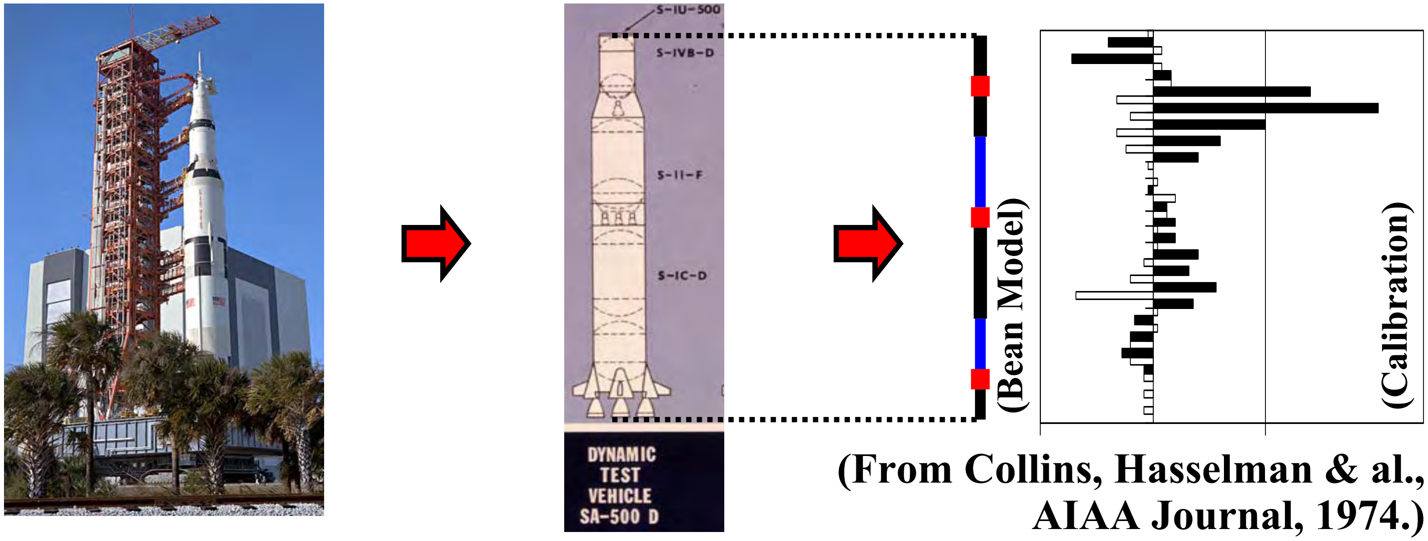
Difficulties of Uncertainty Assessment

- Experimental data sets are sparse and often uncertain.
- Models have distributions on their outputs.
- The unavoidable modeling assumptions provide a false sense of confidence by "hiding" the *lack-of-knowledge*.
- No evidence is available to suggest that these uncertainties follow traditional probability distributions.
- No evidence is available to suggest membership functions, possibility structures, degrees of belief, etc.

Why Do We Make Assumptions?

- **Assumptions enable model-building.**

Reality of Interest **Conceptual Model** **Computational Model**

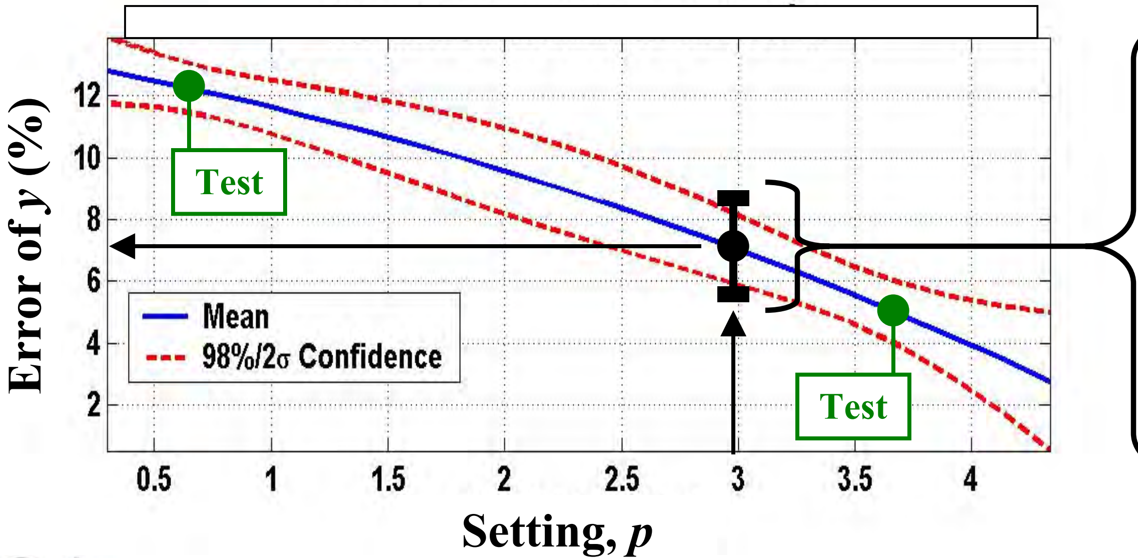


(From Collins, Hasselman & al., AIAA Journal, 1974.)

- **Modeling assumptions *reduce* the uncertainty!**
- **The extent to which modeling assumptions influence the predictions and decisions must be quantified.**

Prediction Accuracy Assessment is Nothing But *Total Uncertainty* Quantification …

- **Instead of reducing the lack-of-knowledge by making an assumption, the modeling uncertainty should be assessed.**
- ***"For the setting of p=3, the simulation can predict y with an accuracy of 7% +/- 1%, at the significance level of 96%."***



The prediction bounds include a quantification of the modeling uncertainty.

"The model is linear."

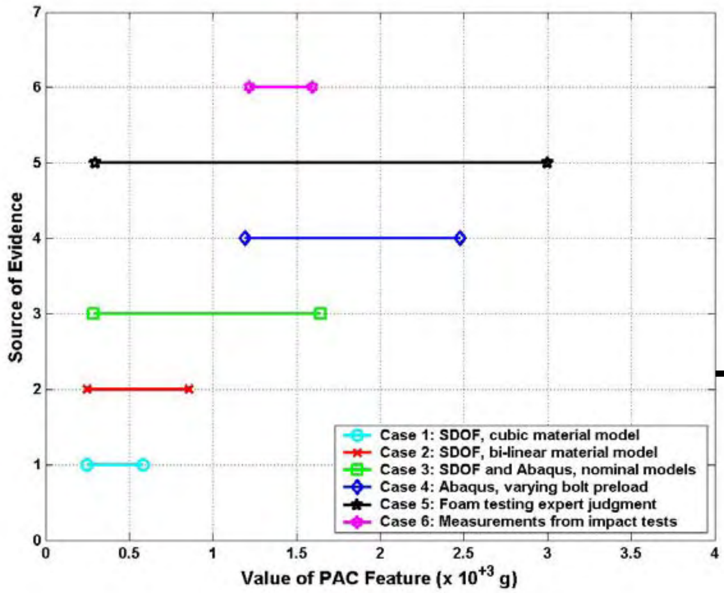
"The model is quadratic."

"The model is cubic."

The Concept of Total Uncertainty

- **Evidence is provided by different models, test data, expert judgment, and a probabilistic high-fidelity simulation. It is combined into a single assessment of *total uncertainty*.**

Collection of Evidence



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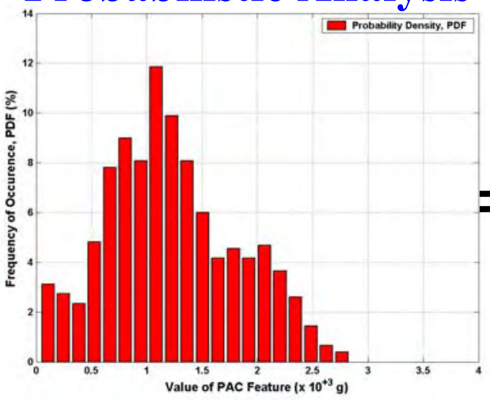
Probabilistic Analysis



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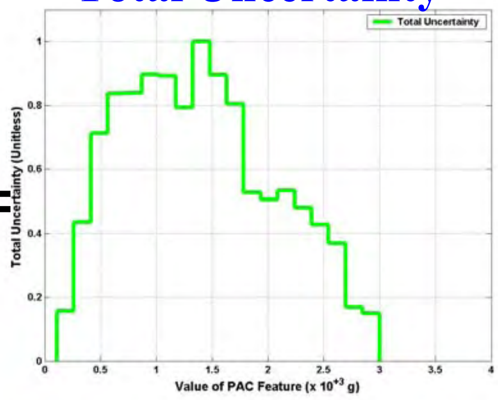
Total Uncertainty



A (Short) List of Open Questions

- How to combine probabilistic models of uncertainty with the General Information Theory (GIT)?
- How to define a metric for model validation?
- How to compute the "margin-to-requirement"?
- How vulnerable are our decisions to everything we do not know (the "unknown unknowns")?
- What is the relationship (if any) between fidelity-to-data, immunity-to-uncertainty, and confidence-of-prediction?

A Few Resources

- ***Uncertainty Quantification and Model Validation (UQMV) sessions at technical conferences in the United States:*** **International Modal Analysis Conference; Structures, Structural Dynamics and Materials Conference; U.S. National Congress in Computational Mechanics.**

- ***SAMO-2004:*** **Los Alamos is hosting the 4th International Conference on Sensitivity Analysis of Model Output (SAMO-2004), March 8-11, 2004, in Santa Fe, New Mexico. Abstract deadline is September 15, 2003. Information at www.samo-2004.org.**

- ***A few resources on V&V:***
  - **The U.S. Department of Defense's Defense Modeling and Simulation Office (www/dmso.mil).**
  - **ASME standard committee on Verification and Validation in solid mechanics (www.usacm.org/vnvcsm).**
  - **Short courses on V&V by Patrick Roache, Bill Oberkampf, and LA Dynamics (www.la-dynamics.com).**