SAND2016-5894C

Exceptional service in the national interest

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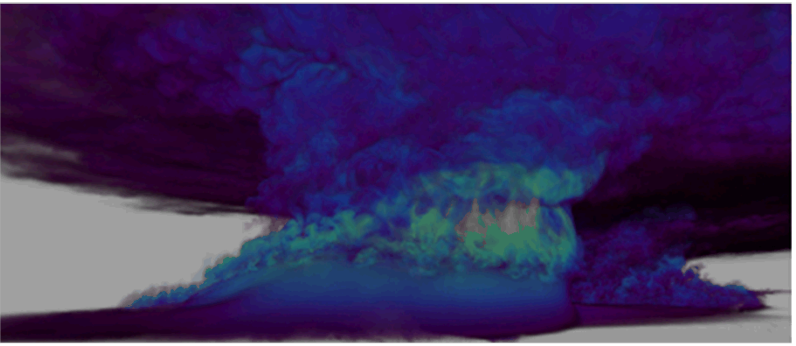

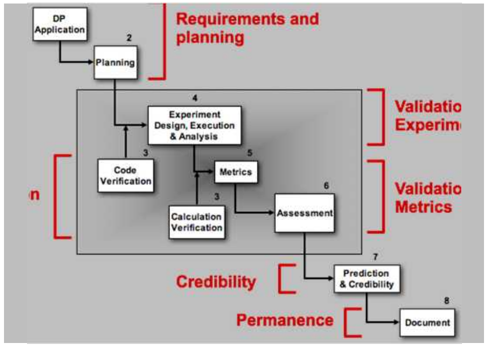

Believable Fake - Credible Simulation for Nuclear Weapon Design

Scott Hutchinson
Senior Manager, Computational Simulation

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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Outline

- CompSim and Me
- What do you believe?
- Simulation
  - Physical Simulation
  - Computational Simulation
- Credible Simulation
  - The Challenges
  - The Approach
  - The Challenges, again
  - The Way Forward
- The Summary

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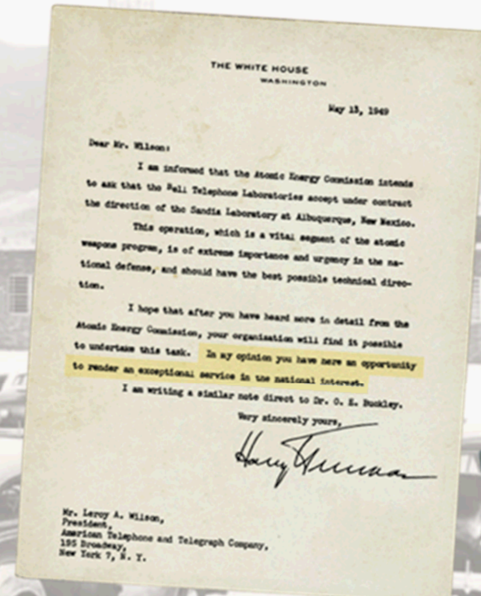
Exceptional service in the national interest

Then….

July 1945: Los Alamos creates Z Division

Non-nuclear component engineering

November 1, 1949: Sandia Laboratory established



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely yours,

Harry Truman

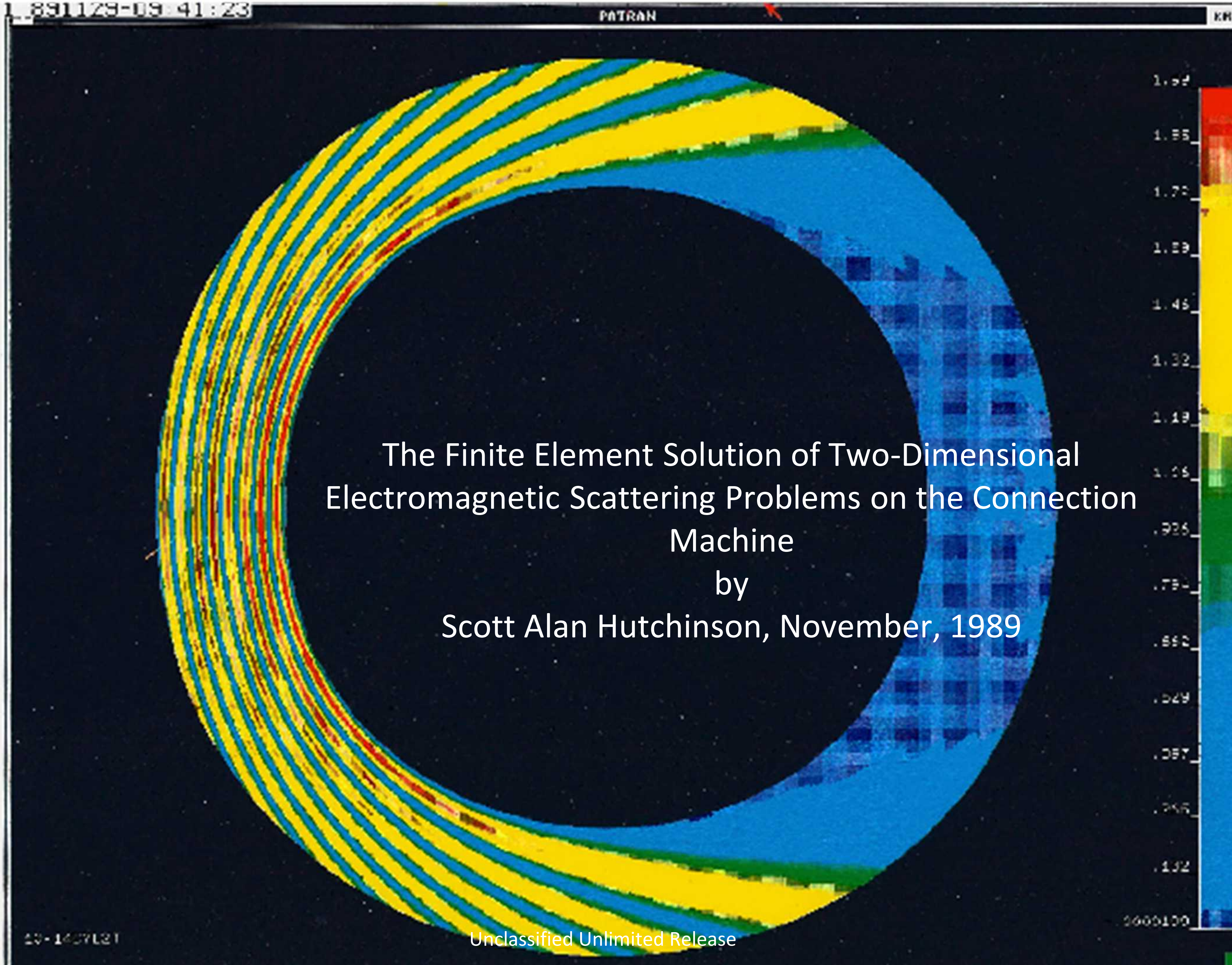
Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

Now….

Core mission in Non-nuclear components of Nuclear Weapons

Addressing the nation's most challenging National Security problems

- USS Iowa (1989)
- TWA Flight 800 Accident (1997)
- Post 9/11 Vulnerability Studies (2001)
- Columbia Space Shuttle Accident (2003)
- I-35W bridge collapse in Minneapolis (2007)
- BP Deepwater Horizon Oil Spill Accident (2010)
- Aircraft Vulnerability (2013)
- Waste Isolation Plant Leak (2014)



The Finite Element Solution of Two-Dimensional Electromagnetic Scattering Problems on the Connection Machine

by

Scott Alan Hutchinson, November, 1989

My background…

$$\nabla \cdot \mathbf{D} = \rho \qquad (1) \qquad \text{Gauss' Law}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad (2) \qquad \text{Gauss' Law for magnetism}$$

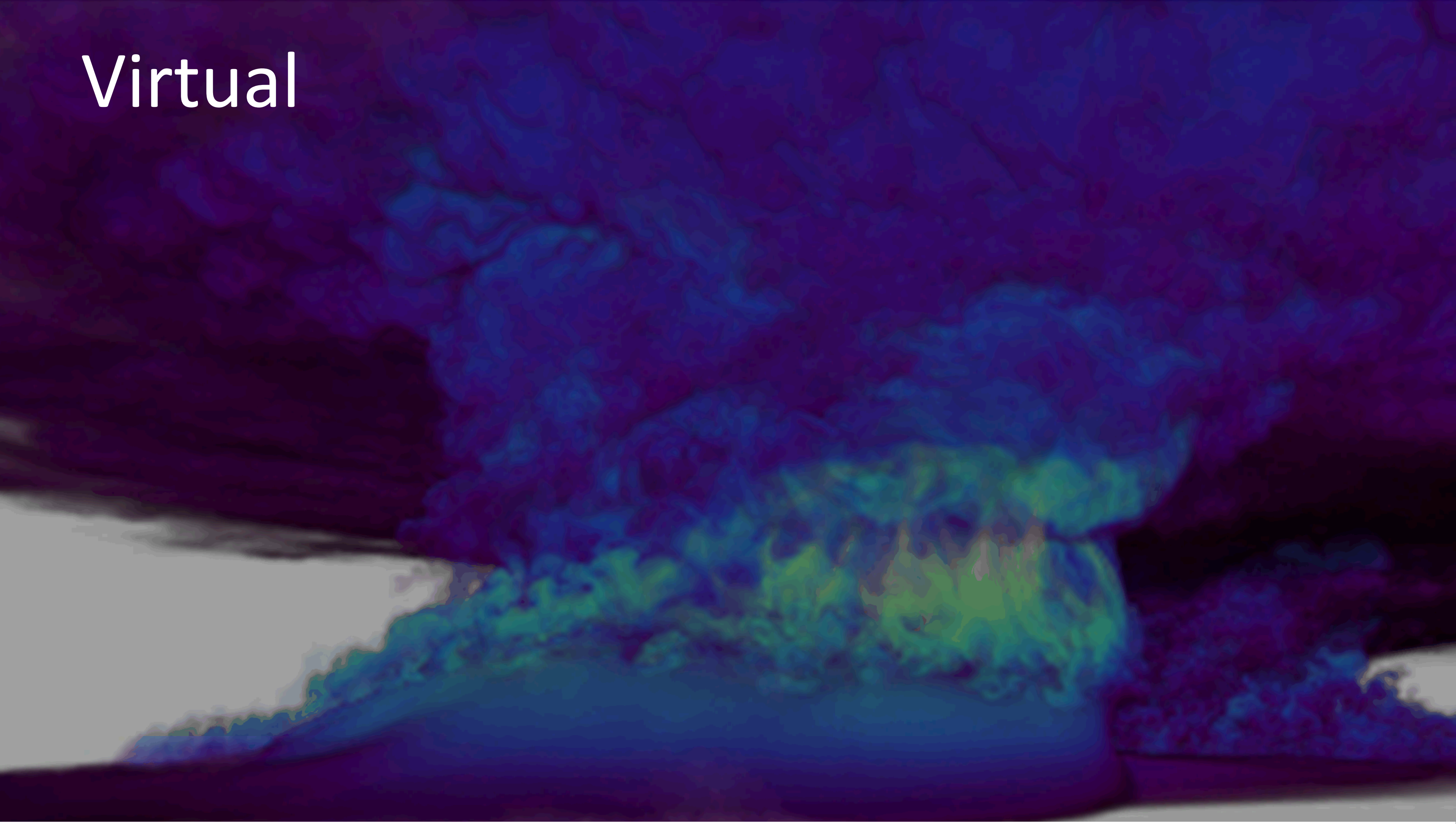
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad (3) \qquad \text{Faraday's Law}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \qquad (4) \qquad \text{Ampère-Maxwell Law}$$

But that's ok…

Credible Simulation

Virtual



Reality …Not

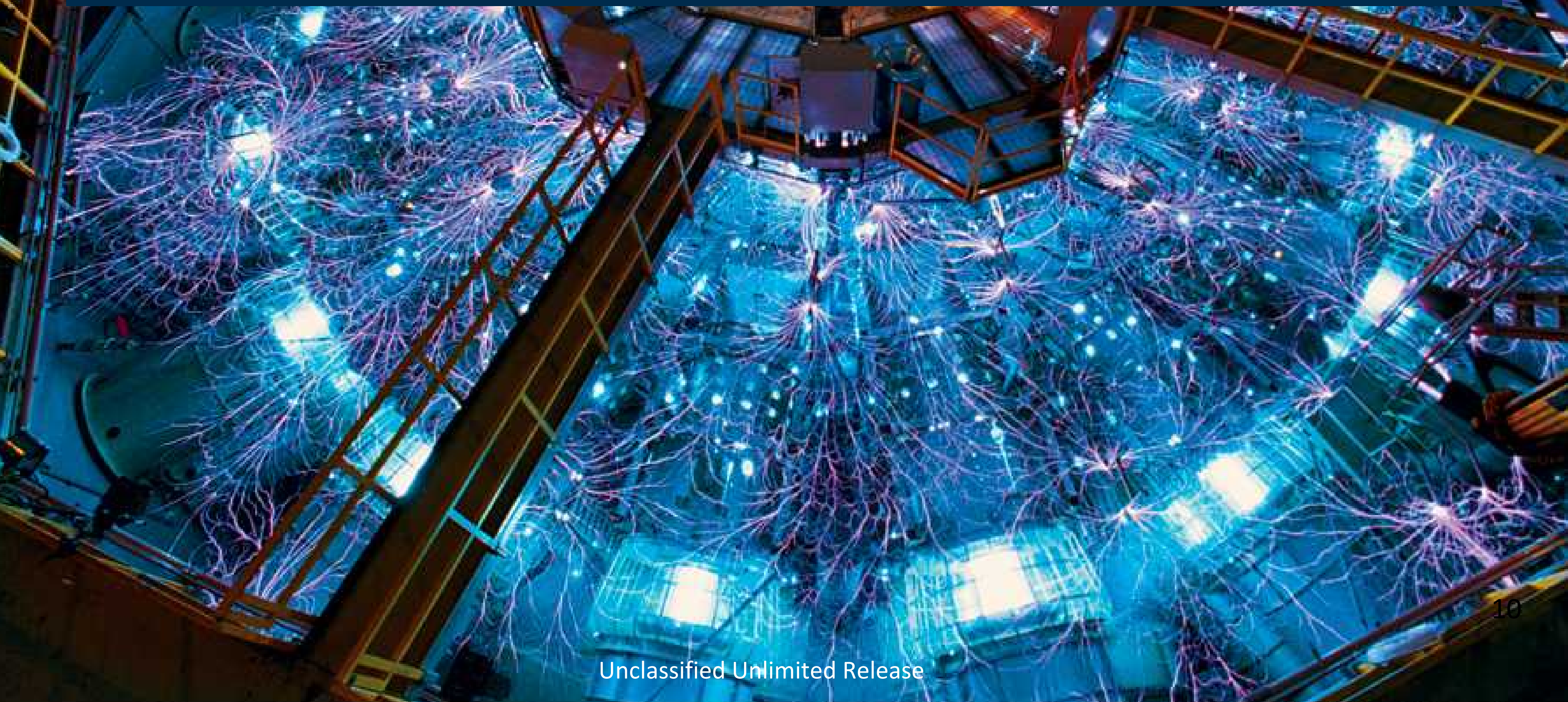
CYBER STORM The 60-kilometer-wide swirling thunderstorm in this simulation spawned the first digitally created long-lived EF5 tornado (bottom, right-center). The 700-meter-wide virtual twister may reveal why some real-life tornadoes linger.
David Bock (University of Illinois at Urbana-Champaign), Leigh Orf (University of Wisconsin), Robert R. Sisneros (University of Illinois at Urbana-Champaign)

But let’s begin by discussing the source of such comparisons, simulation

Two primary types of Simulation upon which we rely:

Physical simulation (PhysSim)

Computational simulation (CompSim)



Quantitative ways of measuring differences

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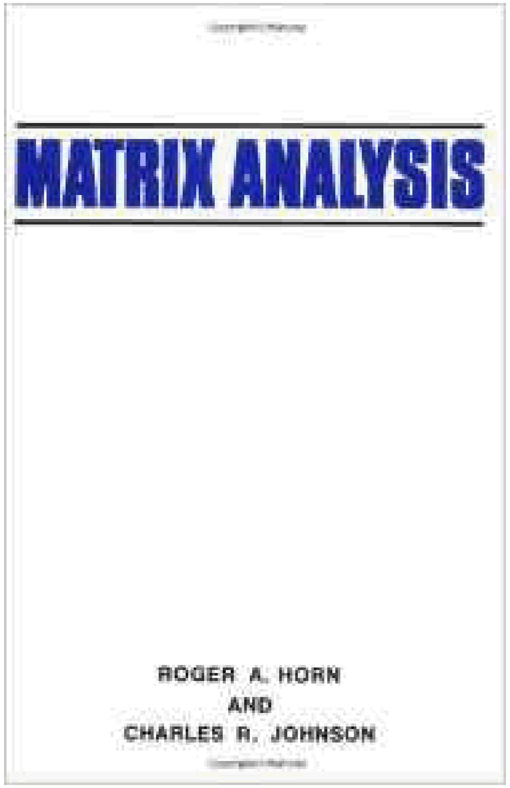
Euclidian Norm: $\|x\| = \sqrt{\sum_j x_j{}^2}$

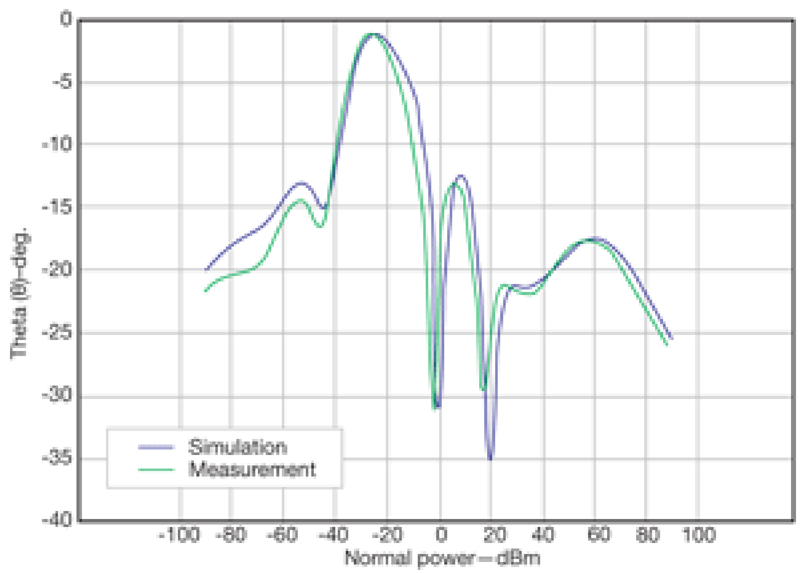
p-Norm: $\|x\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{\frac{1}{p}}$.

Maximum Norm: $\|x\|_\infty = \max\{|x_1|, |x_2|, \ldots, |x_n|\}$

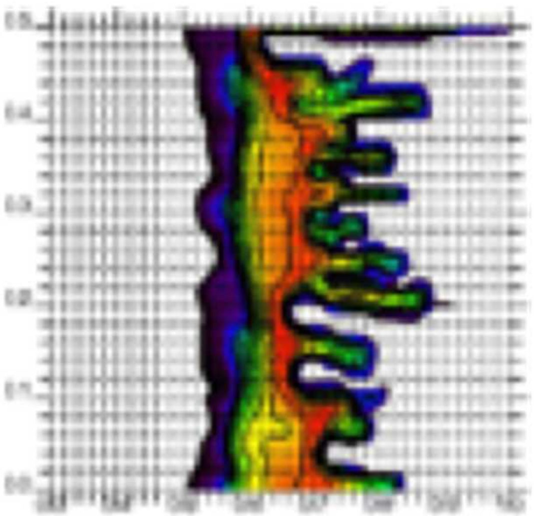


However, computational simulation has introduced new, less rigorous norms…

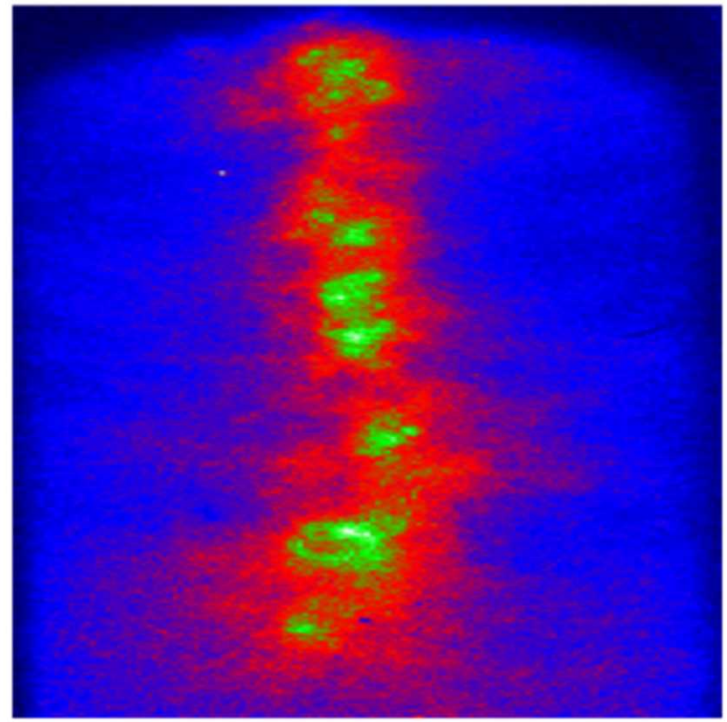
The Viewgraph Norm
(AKA The Eyeball Norm)



The Beauty Contest Norm



2-D r-z shell implosion calculation.



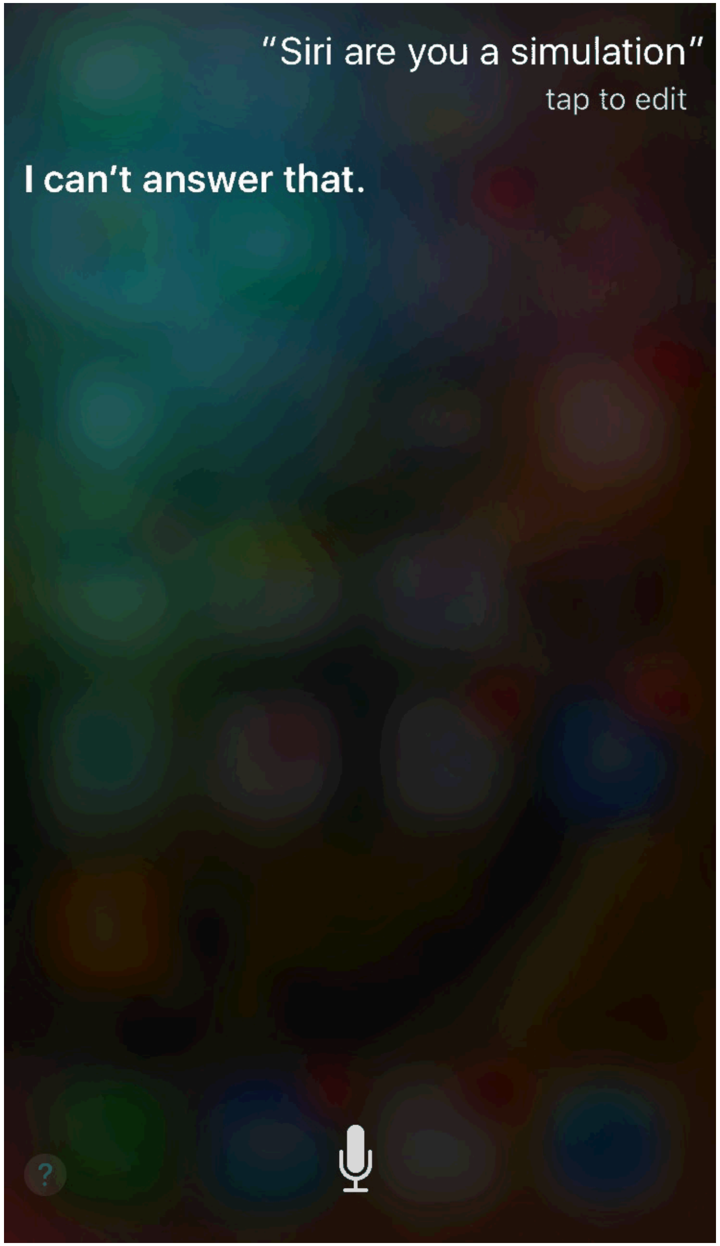
Experimental spectroscopic image of Z-pinch liner stagnation.

Let’s make one thing clear

We never rely on any CompSim alone for supporting any decision

Rather, we have at least three pillars we use for evidence at the system and/or component levels:

- Physical Simulation
  - Field/Flight Tests
  - Lab Tests
- Computational Simulation
- Expert Judgment
  - Subject Matter Experts
  - Peer Reviews
  - Independent Reviews



Simulation: from the Latin *simulare:*

1. *<u>counterfeit</u> or <u>fake</u>*
2. *feint*
3. *imitate, copy*
4. *look like*
5. *pretend (to have/be)*
6. *simulate*

…by definition, then, a simulation is wrong

But, saying it is wrong is useless, knowing why it is wrong is the point…

or put positively:

Why is your simulation accurate or useful?

Credibility:

The quality, capability, or power to elicit belief

Are we ready for the challenge?

If called upon, how do we defend our results?

What evidence is necessary to support our claims?

It depends on the questions being answered by the decision maker using the simulation results…

…AND the risk associated with the decision being wrong

Courtesy of Walt Witkowski, Sandia, 2016

Let us start at the beginning…

(the beginning of ASC at DOE/NNSA, that is)

Advanced Simulation & Computing (ASC):

The purpose of computing is to provide

“high-performance, full-system, high-fidelity-physics <u>predictive</u> codes to support weapon assessments, renewal process analyses, accident analyses, and certification.”

(DOE/DP-99-000010592)

There's a new word in here: predictive

(I don't really want to look up another definition)

So, we're supposed to be doing *predictive Computational Simulation*? What does that mean?

- Predictability – A technical concept, conventionally arising in the consideration of complex systems. I.e. as in "predict the stability of the solar system" or "predict the evolution of a chaotic system."
- Predictive Capability – in particular a computational capability with some (rigorous?) basis for credible interpolation or extrapolation of current knowledge, for example experimental data.

Courtesy of Tim Trucano, Sandia, 2006

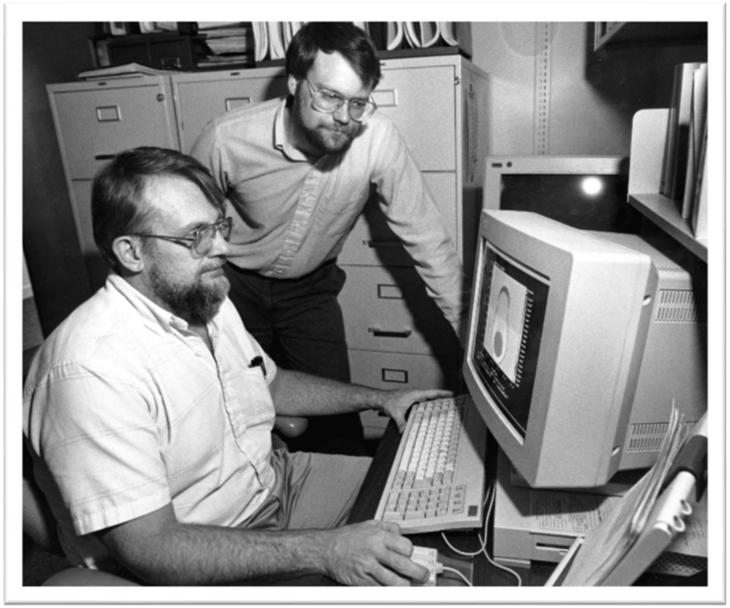
Do you trust the simulation?
Can you trust the simulation?

Three reasons you may not wish to bet your life on a simulation:

1. Wrong physics
2. Wrong numerics
    - Wrong math, algorithms, software, wrong inputs, etc.
    - Lousy numerical accuracy

3. Wrong use of the results*

(* Especially scary!)



Courtesy of Tim Trucano, Sandia, 2006

According to the NNSA/ASC Program:

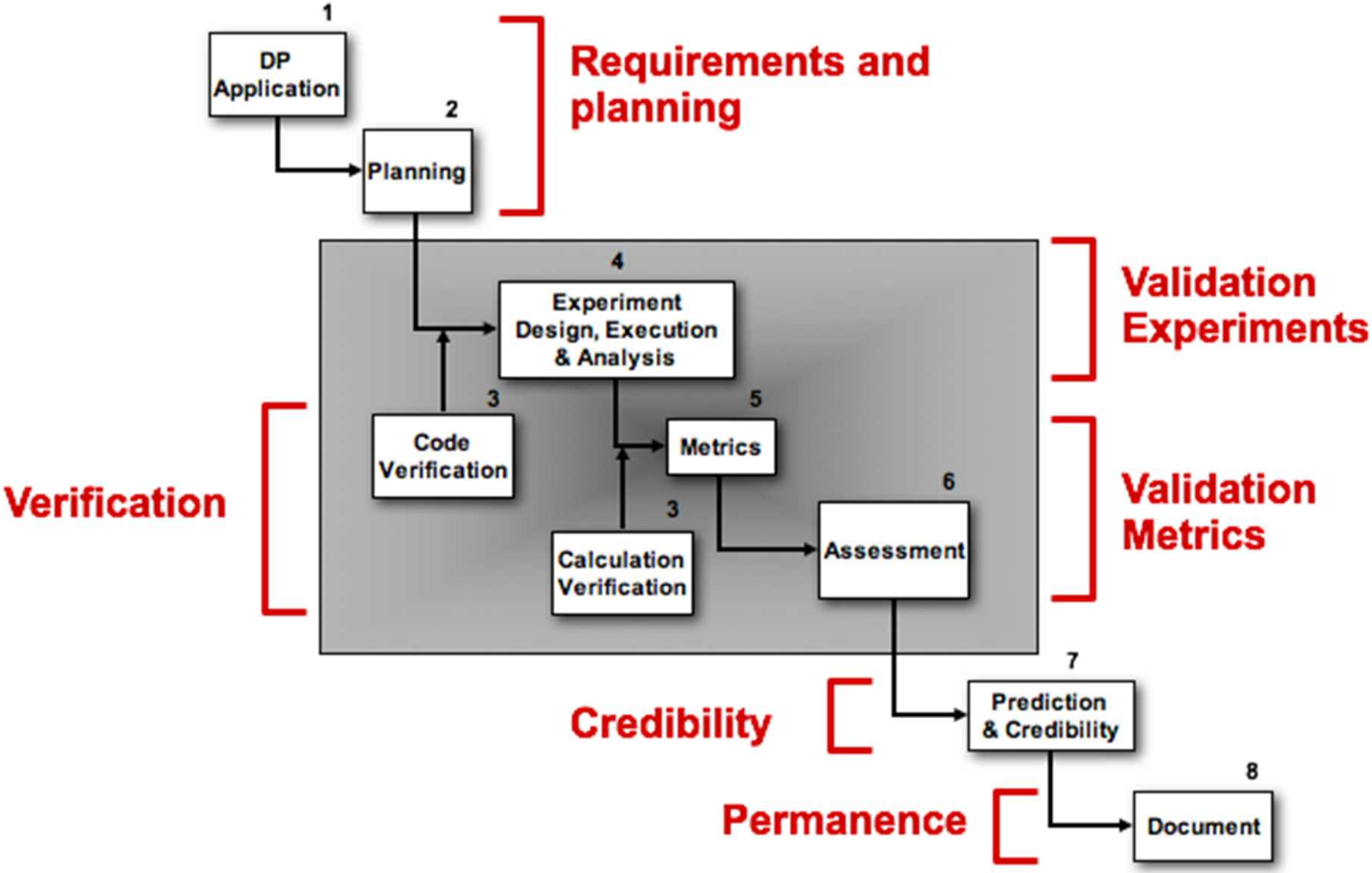
- Verification: The process of confirming that a computer code correctly implements the algorithms that were intended.

- Validation: The process of confirming that the predictions of a code adequately represent measured physical phenomena.

Verification – Are the equations solved correctly? (Math)
Validation – Are the equations correct? (Physics)

What goes into Credible Simulation?

Like any good government entity, we have a process…



And out of this process we have developed a lot of subprocesses and tools

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VERIFICATION™ VALIDATION

percept

QMU

Predictive Capability Maturity Model

FCT

PIRT

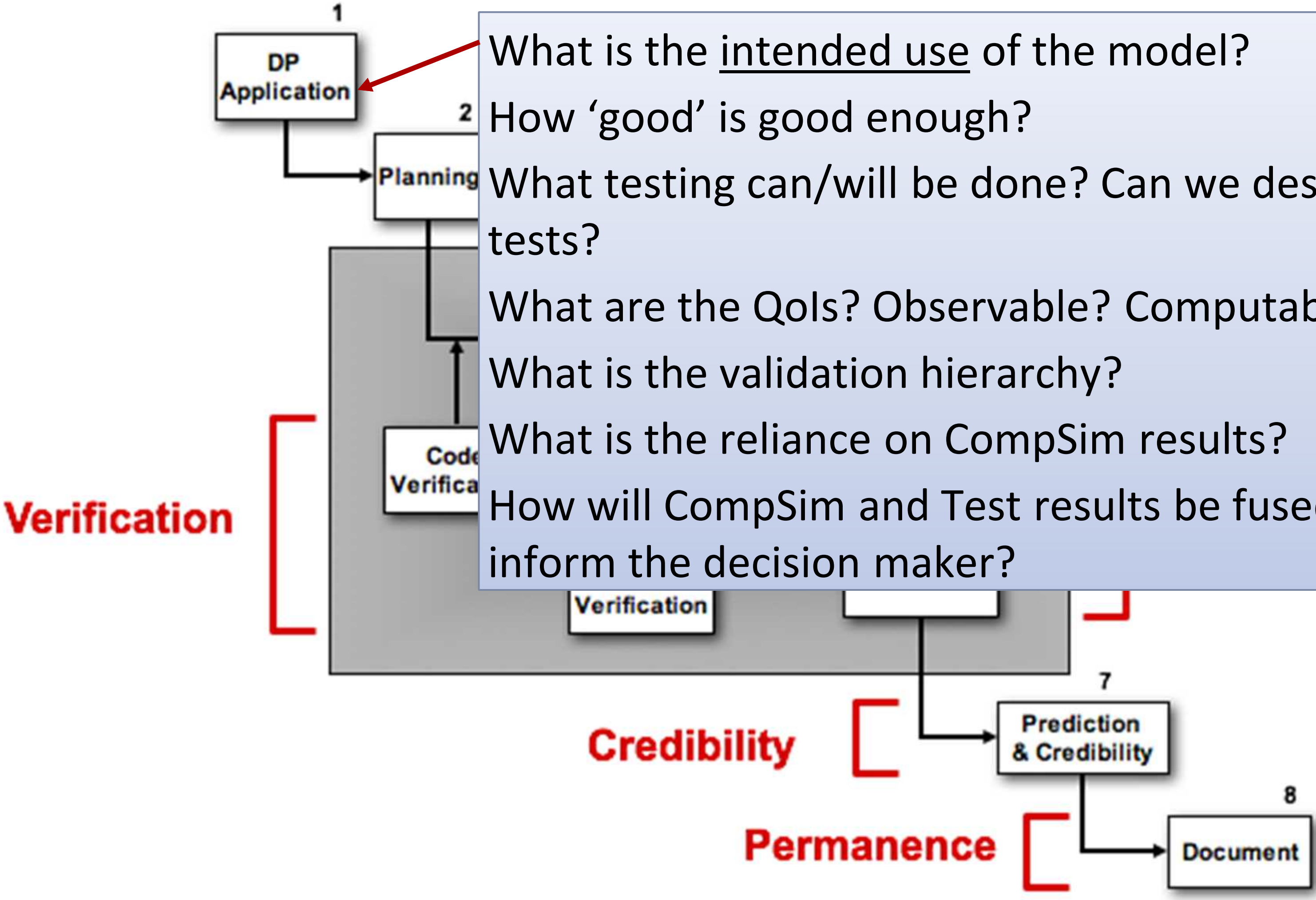
Uncertainty Quantification

…and more, much more…

Let's take a brief walk through this process

Courtesy of Walt Witkowski, Sandia, 2016

Understand the Application and Requirements



- What is the <u>intended use</u> of the model?
- How ‘good’ is good enough?
- What testing can/will be done? Can we design tests?
- What are the QoIs? Observable? Computable?
- What is the validation hierarchy?
- What is the reliance on CompSim results?
- How will CompSim and Test results be fused to help inform the decision maker?

Assess Capabilities, Identify Gaps & Prioritize Work

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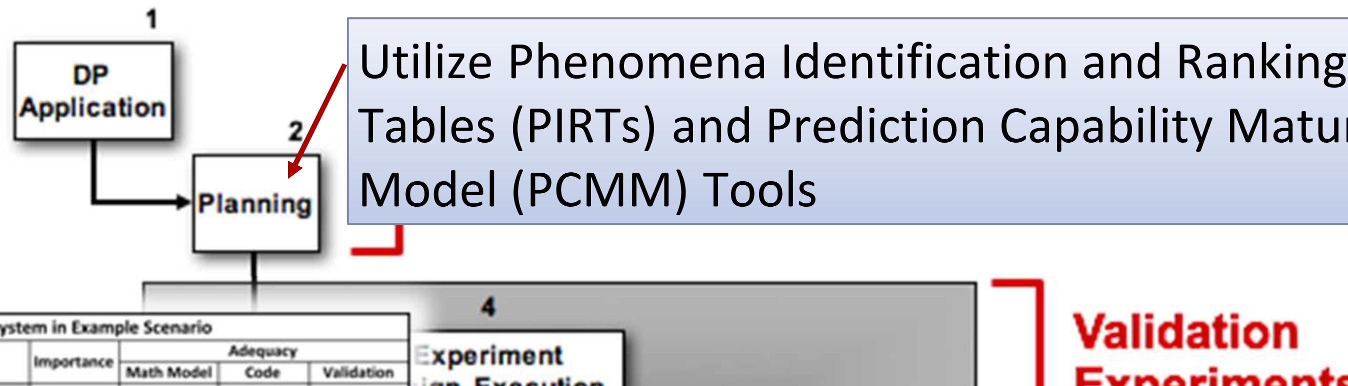
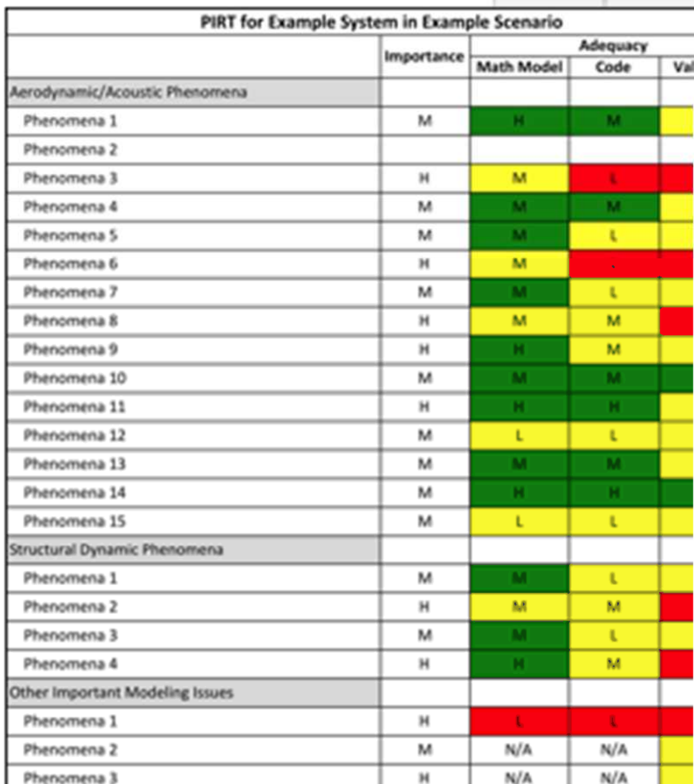
Utilize Phenomena Identification and Ranking Tables (PIRTs) and Prediction Capability Maturity Model (PCMM) Tools



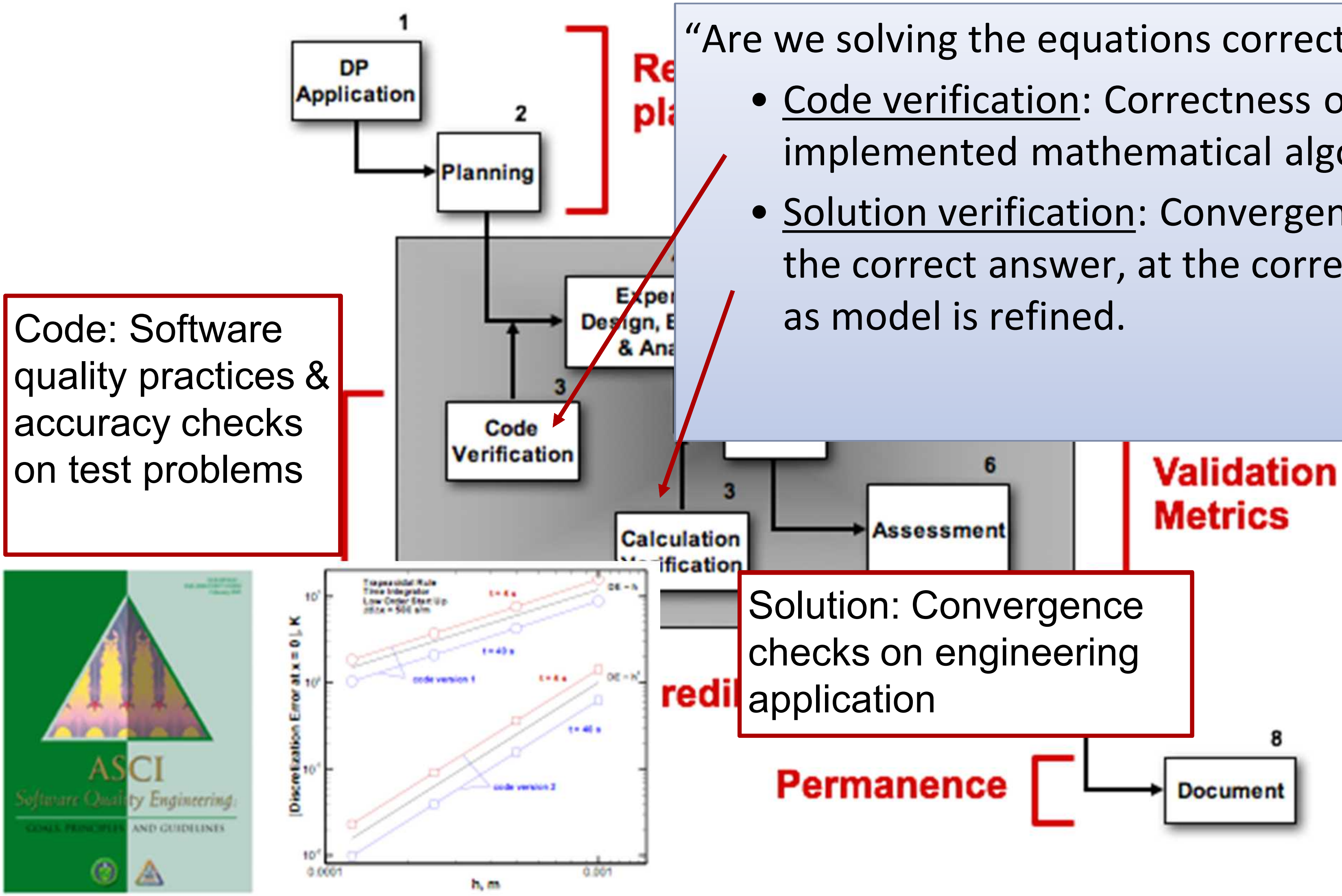


PIRT for Example System in Example Scenario

	Importance	Adequacy		
		Math Model	Code	Validation
Aerodynamic/Acoustic Phenomena				
Phenomena 1	M	H	M	
Phenomena 2				
Phenomena 3	H	M	L	
Phenomena 4	M	M	M	
Phenomena 5	M	M	L	
Phenomena 6	H	M		
Phenomena 7	M	M	L	
Phenomena 8	H	M	M	
Phenomena 9	H	H	M	
Phenomena 10	M	M	M	
Phenomena 11	H	H	H	
Phenomena 12	M	L	L	
Phenomena 13	M	M	M	
Phenomena 14	M	H	H	
Phenomena 15	M	L	L	
Structural Dynamic Phenomena				
Phenomena 1	M	M	L	
Phenomena 2	H	M	M	
Phenomena 3	M	M	L	
Phenomena 4	H	H	M	
Other Important Modeling Issues				
Phenomena 1	H	L	L	
Phenomena 2	M	N/A	N/A	
Phenomena 3	H	N/A	N/A	

ELEMENT \ MATURITY	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and BCs	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built", e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&C) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have an unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive sensitivity analyses conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

Verification Activities



"Are we solving the equations correctly?"

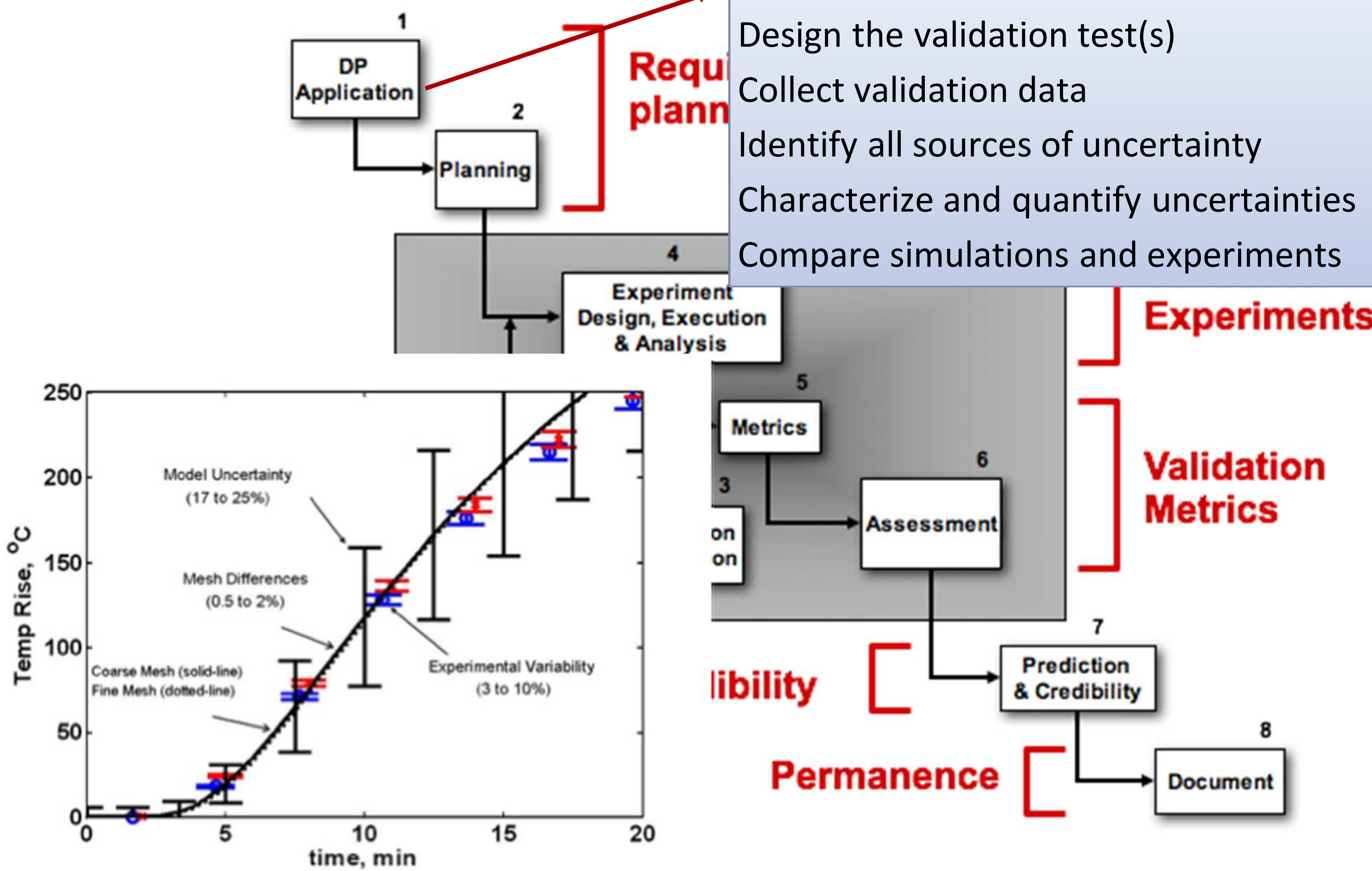
- Code verification: Correctness of implemented mathematical algorithms.
- Solution verification: Convergence to the correct answer, at the correct rate, as model is refined.

Code: Software quality practices & accuracy checks on test problems

Solution: Convergence checks on engineering application

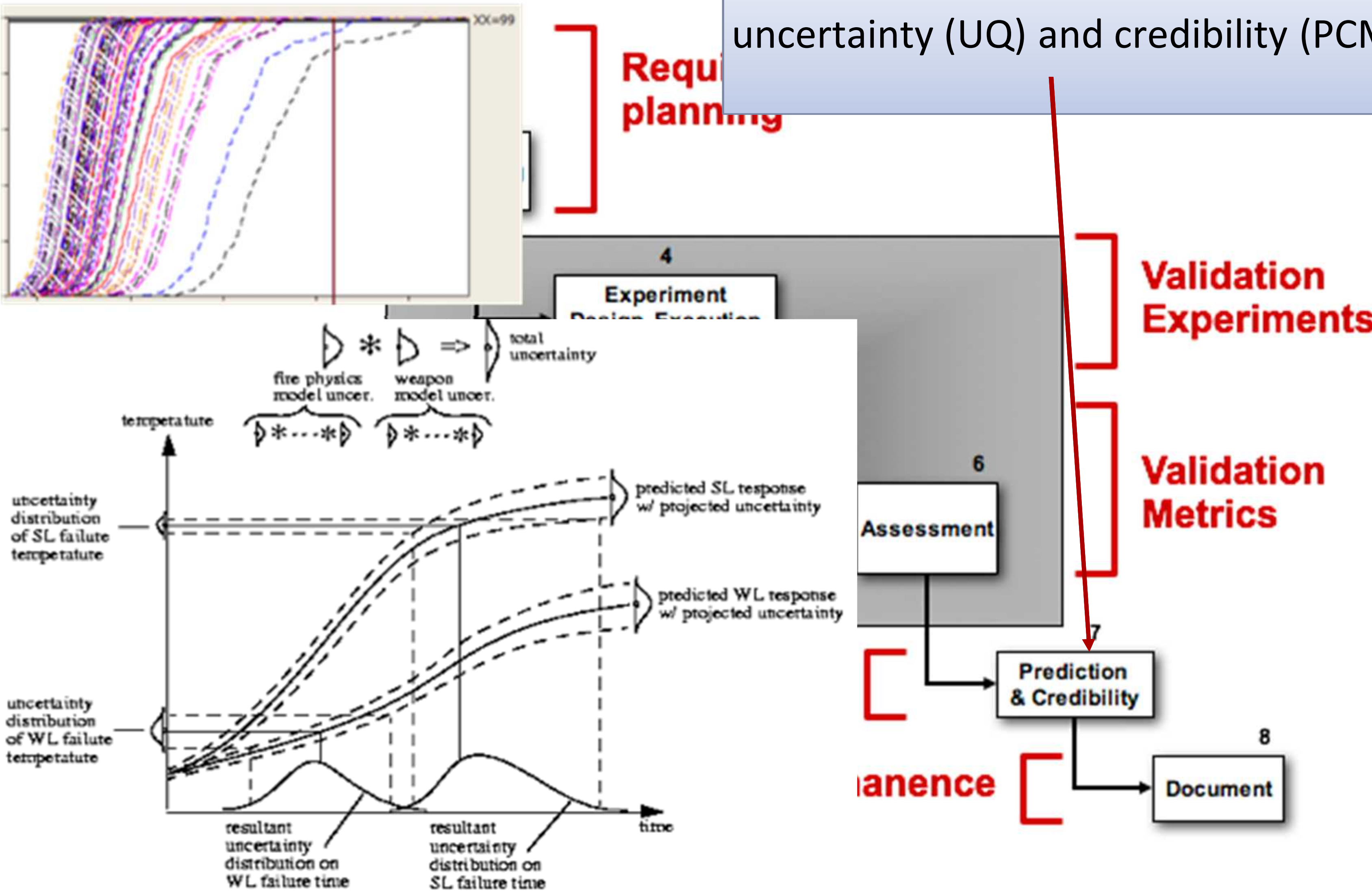
Validation/UQ Activities

- Develop validation metrics and criteria
- Design the validation test(s)
- Collect validation data
- Identify all sources of uncertainty
- Characterize and quantify uncertainties
- Compare simulations and experiments

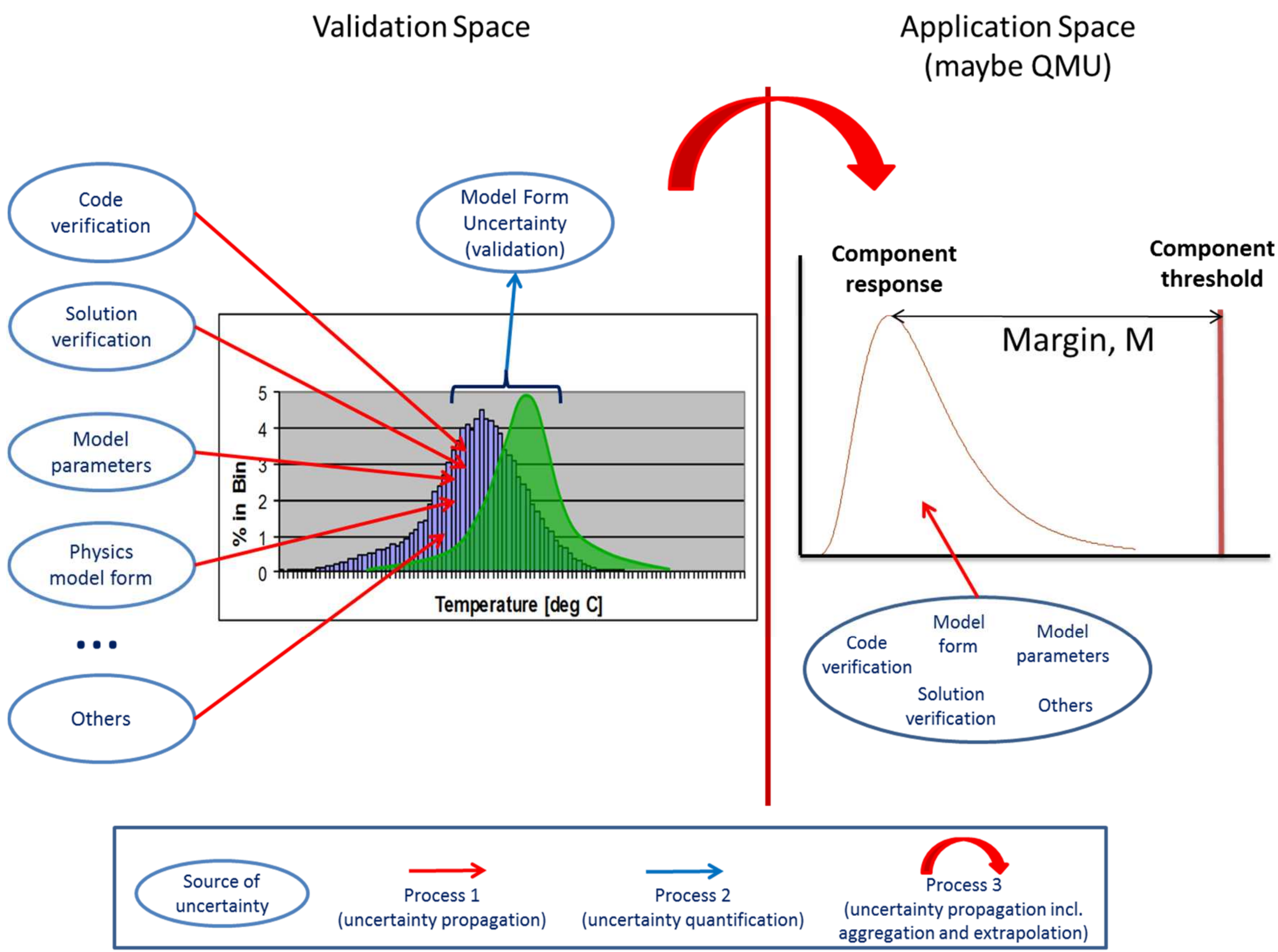


Predictions

Predictions with assessments of uncertainty (UQ) and credibility (PCMM)



From validation to application space



Did that seem like a lot of work?

It gets worse - this really is a “NP-Hard” problem

For example, we've written application tools to help with V&V: Feature Coverage Tool

Now we have to V&V this tool as well!

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This “credible simulation” thing isn’t for the faint of heart!

But we can still succeed!

Three key principles for to help us scope Credible Simulation:

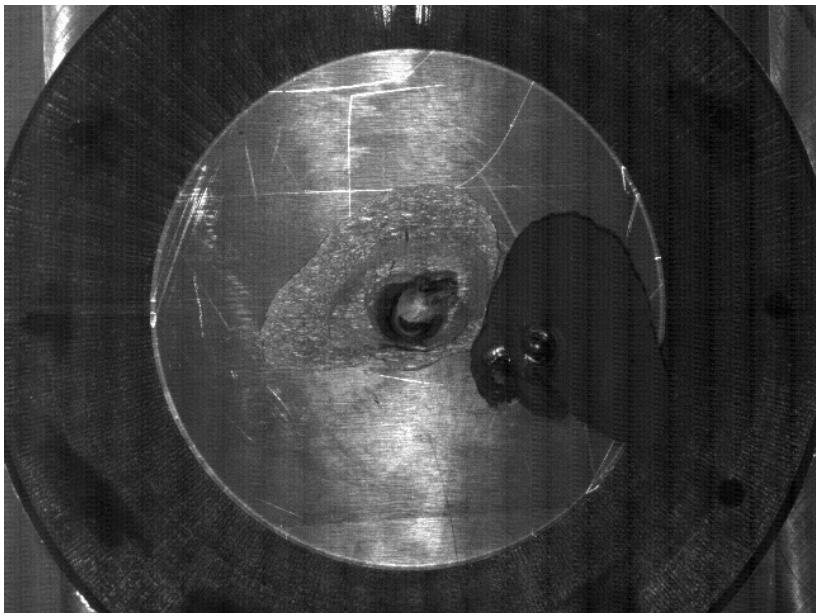
1. Best-estimate plus uncertainty (*how incorrect is your result?*)
2. Sufficiency of process and evidence for the intended use (*is your result correct enough?*)
3. Judgment (*how do you know?*)

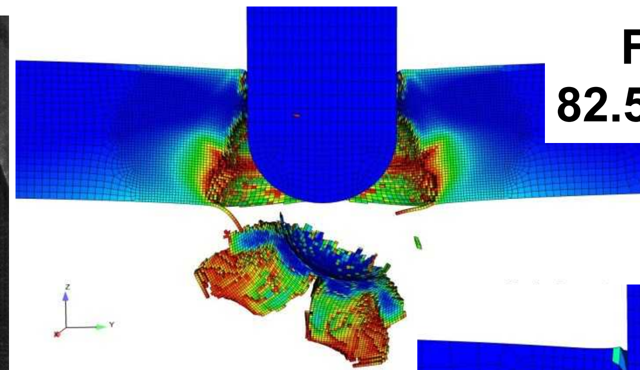
Let’s look at a brief example

Example: Failure Predictions for Abnormal Mechanical Environments

Principal Objective

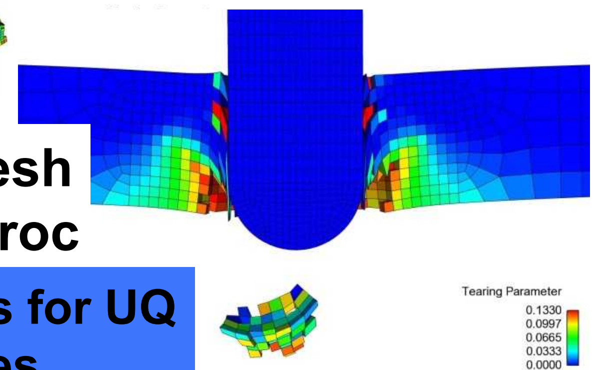
Assess predictions of the minimum penetration velocity using Sierra/SM w/tearing parameter as the failure criterion by comparing to test data.





Fine Mesh
82.5 hrs/48 proc

Coarse Mesh
9.5 hrs/4 proc



Used 100 FEs for UQ analyses

Typically, we can only afford to use a 'coarse' mesh when many function evaluations are involved! Are these models still valuable? Why do we believe in them? What error do they carry with them?

Credibility and Verification Activities

MATURITY / ELEMENT	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
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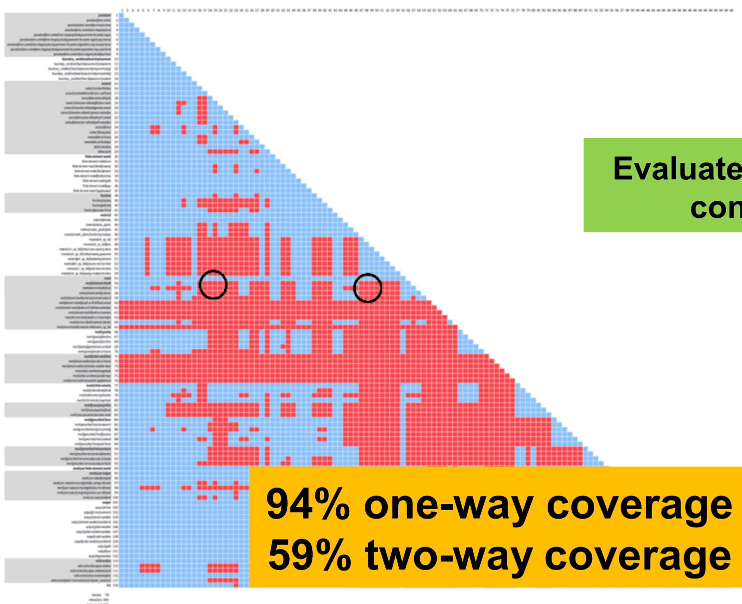
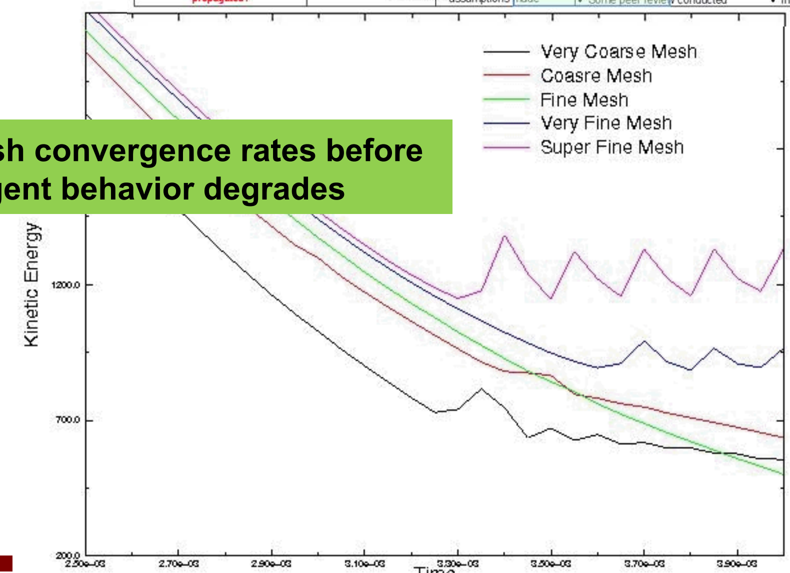
Phenomena	Consensus Importance	Adequacy Math Model	Adequacy Sierra/SM Code	Adequacy Validation
Large elastic-plastic deformation of metals	H	H	M	M
Ductile material failure	H	M	M	L
Contact	H	H	M	M
Friction between punch and test item	M	M	M	L
Enforcement of boundary conditions	L	H	H	L
Inertial loads	H	H	H	M

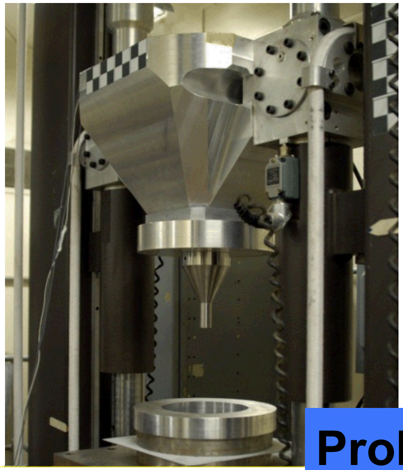


94% one-way coverage
59% two-way coverage

Evaluate mesh convergence rates before convergent behavior degrades



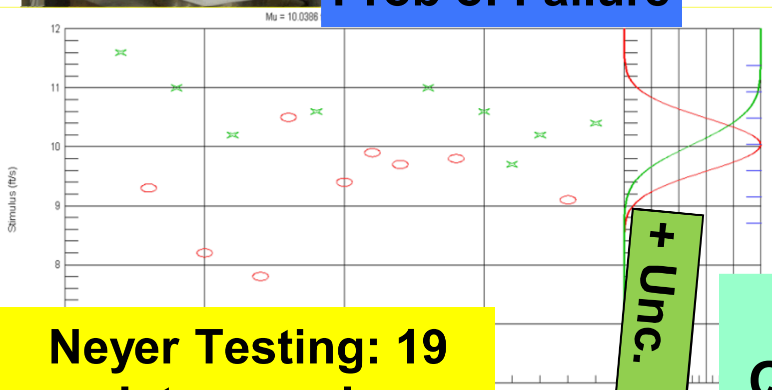
Validation Activities



Uncertainties to Model

Sensitivity analysis helped identify important factors → reduce scope

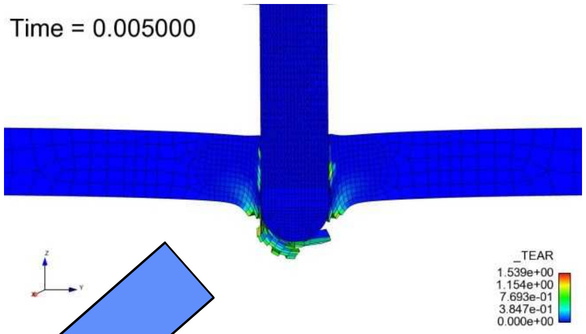
Prob of Failure



Neyer Testing: 19 plate samples

<u>Experimental Uncertainties</u>

- Bungee force
- Friction (punch and plate/tube)
- Velocity measurement
- Material variability-> characterization process



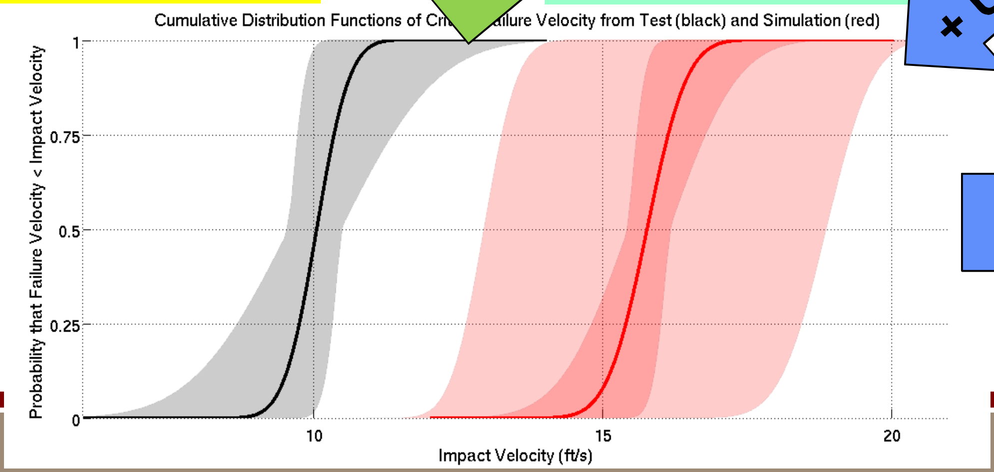
<u>Numerical Uncertainties</u>

- Discretization Error
- Algorithmic parameters

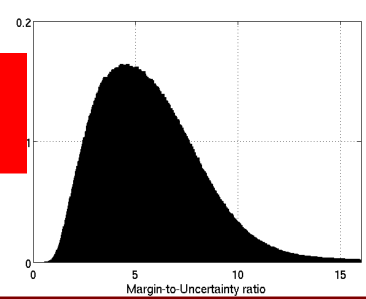
+ Unc.

Uncertainty Quantification

+ Uncertainties



Validation Metrics



What is Model Credibility for Prediction?

An overall assessment of the adequacy (is or is not adequate) of the model for an application based on evidence – *in the end, this is a judgment*

Courtesy of Rich Hills, Sandia, 2015

What Type of Evidence?

<u>Quantitative</u> - results from validation and other relevant experiments, grid convergence studies, sensitivity analysis

<u>Qualitative</u> – structured expert opinion (PIRT, PCMM, internal and external review panels)

Courtesy of Rich Hills, Sandia, 2015

How is this different from validation?

Validation assesses models at the conditions of the validation experiments

Credibility considers the adequacy (a softer assessment) of the model for conditions other than those tested

Courtesy of Rich Hills, Sandia, 2015

There is Irreducible Subjectivity in all of this

People and their Expert Judgment Matter

Summary Points

- Never rely on CompSim alone
- We must understand the intended use of CompSim
- We need practical, graded approaches
- Use CompSim results along with credibility evidence and the associated risks/limitations
- This all holds for physical-simulation credibility as well
- Supporting Credibility must start at the beginning
- Peer reviews are essential
- Expertise (People) is more essential

2120	1054	23091992	0
Approximate number of world-wide nuclear tests	Approximate number of US nuclear tests	Date of last US nuclear test	Number of US nuclear tests since 1992

When it comes to Nuclear Weapons,
"Sorry, my bad"
doesn't cut it.

We are using Computational Simulation more and more to help ensure this never, ever happens.

Our Simulation results must be Credible

Are your simulations credible?

THANK YOU!