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(View-graph Presentation)

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Validation of Composite Models

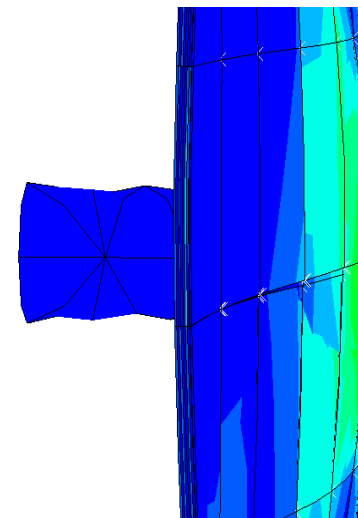


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Abstract

VALIDATION OF COMPOSITE MODELS

The presentation is an overview of concepts, definitions, and technology developed at the Los Alamos National Laboratory in support of Verification and Validation (V&V) activities. An application of V&V to the simulation of projectile impacts against multi-layered composite plates is presented. The goal of the application is to develop a predictive capability to model and simulate the vibration, impact response, and damage propagation characteristics of composite plates in support of structural health monitoring and damage prognosis. After verifying some implementation aspects of the code, mesh convergence studies are conducted. Effect screening is performed to restrict the input parameters to the most significant ones in terms of controlling how predictions of the code vary. All sources of uncertainty, which include modeling assumptions, are propagated through the numerical simulations to estimate the area of between-ply delamination due to projectile impact at various velocities.

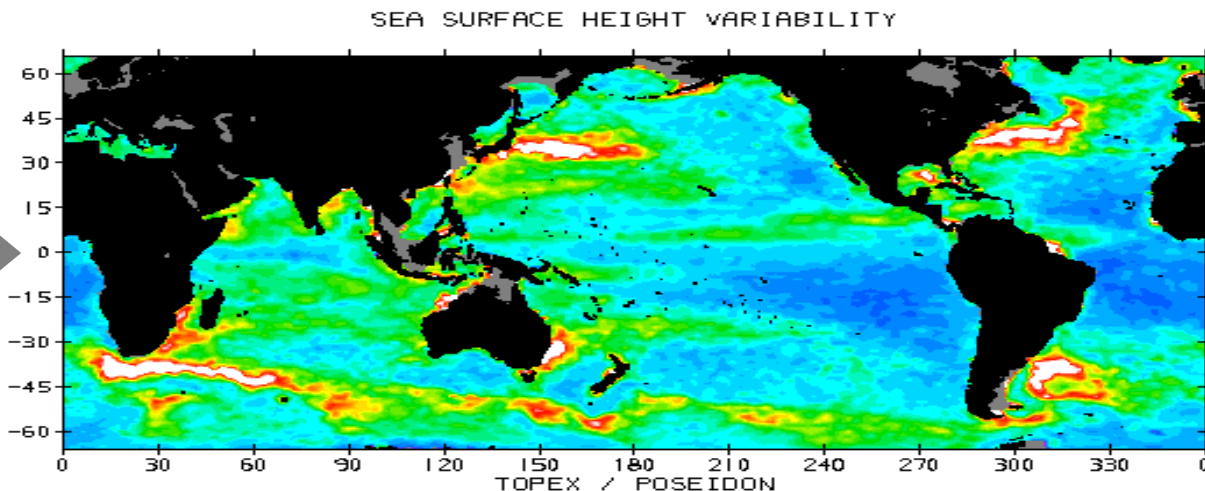
(Presentation approved for unlimited, public release on August 21, 2007, LA-UR-07-5688, Unclassified.)

Outline

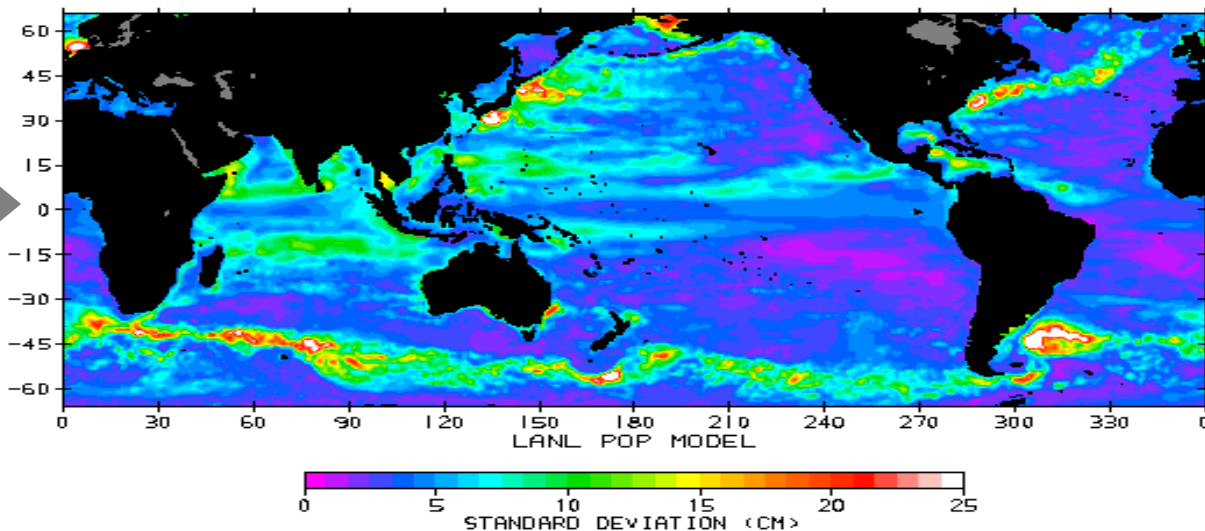
- What does it mean to be predictive?
- Elements necessary to achieve “*predictability*”
- A few lessons learned (as always the hard way ...)
- An application to the validation of composite models
- Closure

Let's Start ... Is This "Validation"?

Observation of the TOPEX/Poseidon Satellite



Calculation of the LANL/POP Simulator (~ 2002)



What Are Verification & Validation?

- **Verification**: *“The process of determining that a computational model accurately represents the underlying mathematical model and its solution.”*

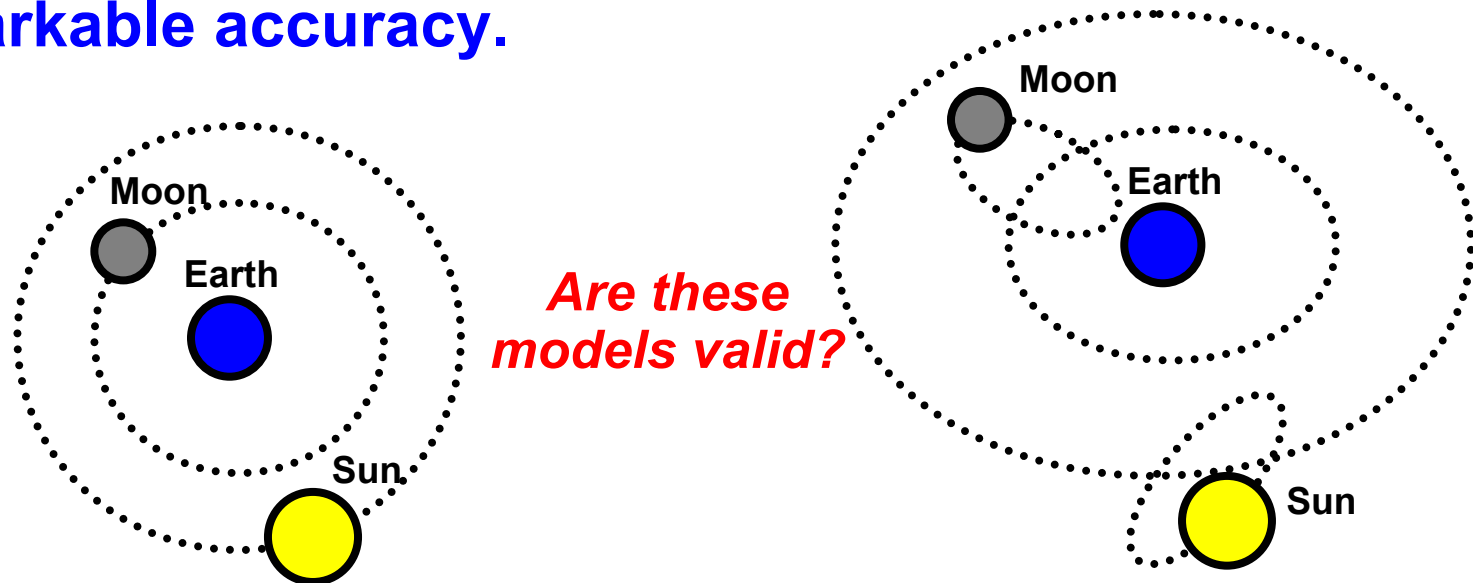
“Stability + Consistency → Convergence.”

(Equivalence theorem of Peter Lax; Comm. in Pure and Applied Mathematics, 1954.)

- **Validation**: *“The process of determining the degree to which a computer simulation is an accurate representation of the real world, from the perspective of the intended uses of the model.”* — U.S. DoD, DoE
- *“The substantiation that a model within its **domain** of applicability possesses a satisfactory range of accuracy consistent with the **intended applications** of the model.”* — S. Schlesinger (1979)

An Example: Greek Astronomy

- These models dominated Western astronomy for over 2,000 years, reproducing the observation of planet positions and predicting the cycles of seasons with remarkable accuracy.



— Pythagoras & Aristotle (~500 BC)

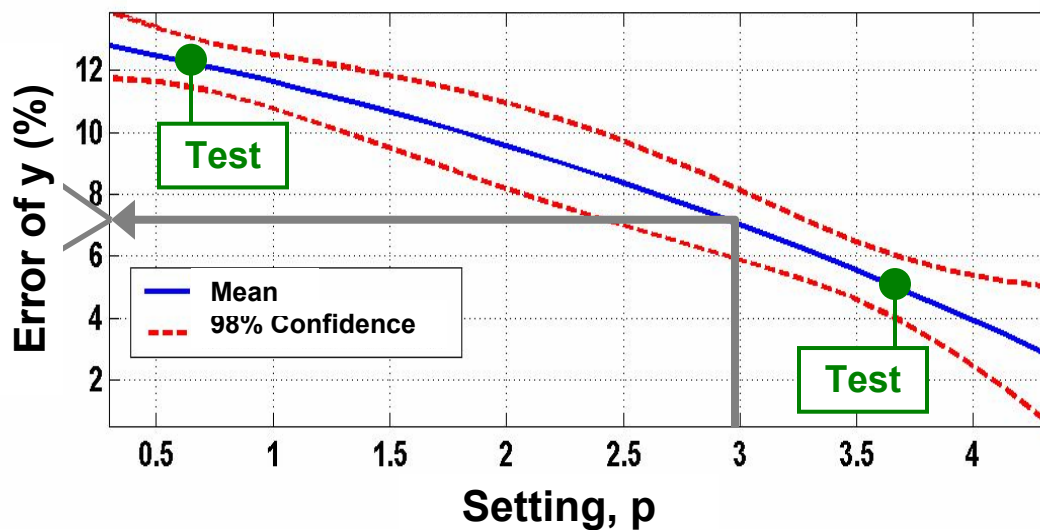
— Ptolemy (~300 BC)

- According to the definition, the answer is “yes:” they are validated for their intended purpose, which was to predict the cycle of seasons for growing crops.

What Does “Predictive” Mean?

- The status of “*predictive capability*” is achieved when, in addition to assessing prediction accuracy, the effect of *all* sources of uncertainty on predictions is quantified. (And it is done so possibly away from settings that have been tested experimentally.)

“For the setting of $p = 3$, the model can predict y with an accuracy of 7% +/- 1%, at the 96% significance level.”



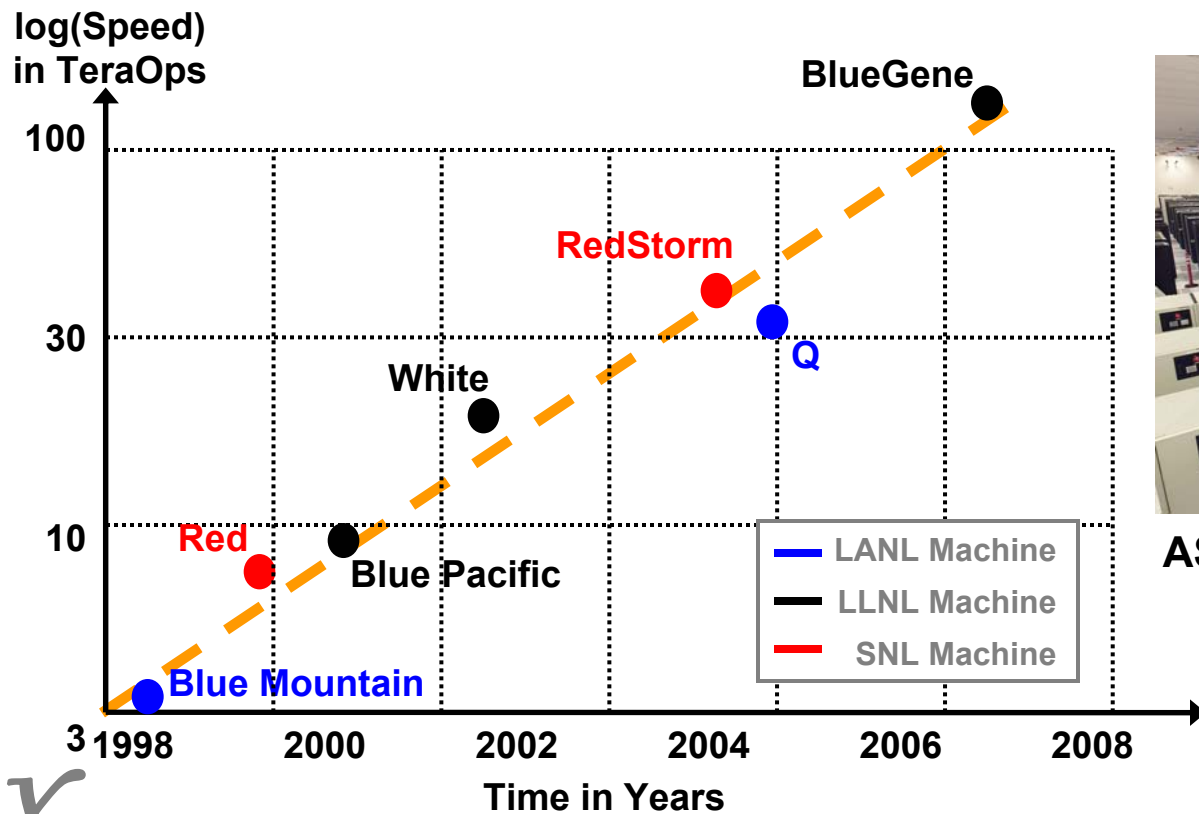
— Systematic bias between predictions and measurements
 - - - Effect of uncertainty on prediction error

Outline

- What does it mean to be predictive?
- **Elements necessary to achieve “predictability”**
- A few lessons learned (as always the hard way ...)
- An application to the validation of composite models
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Computing Resources

- Within the last decade, the formidable development of computing resources has made TeraFLOP computing a reality at Los Alamos (LANL), Livermore (LLNL), and Sandia (SNL) National Laboratories.



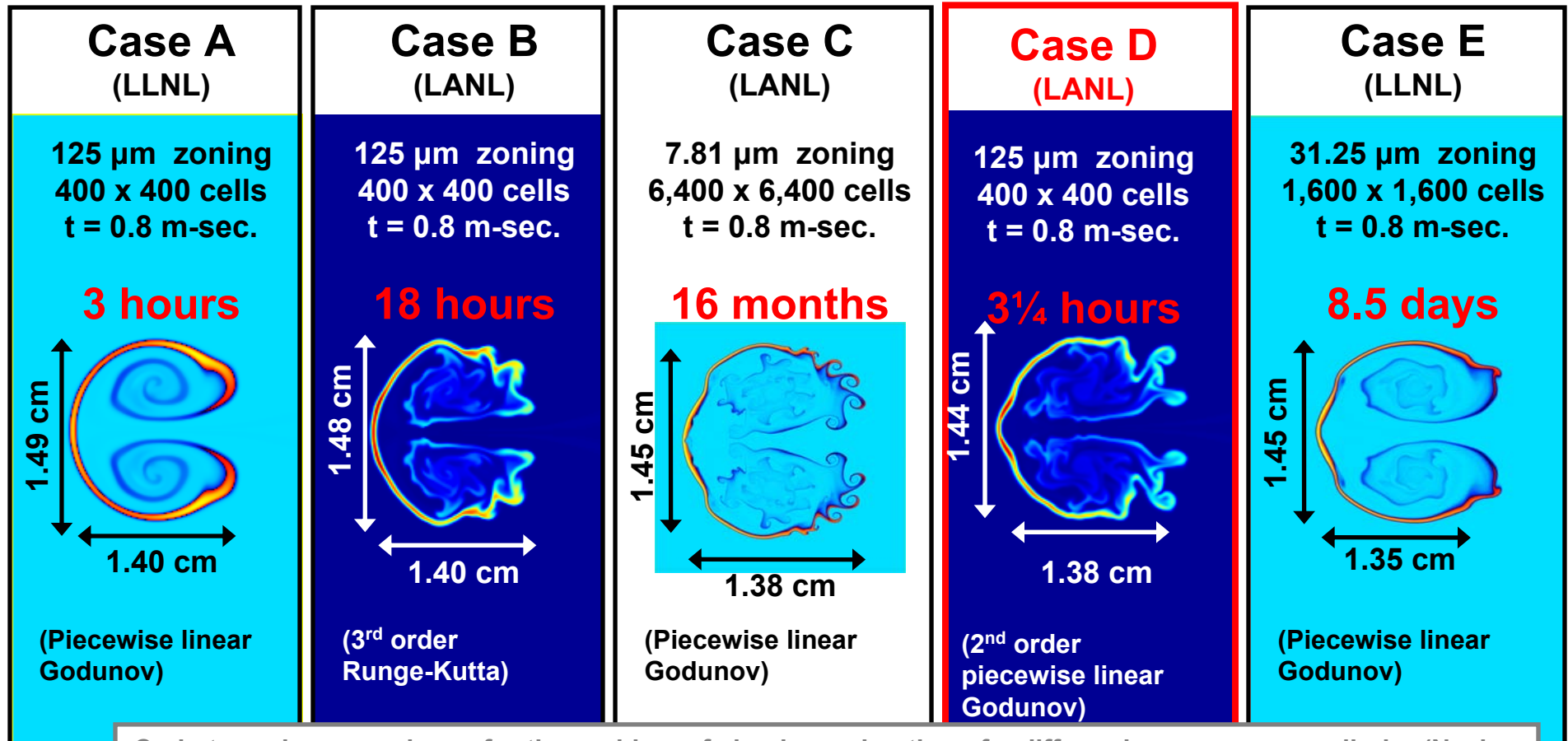
ASC Q at Los Alamos (Nov. 2002)

1 TeraFLOP = 10^{+12} FLOPS
 1 PetaFLOP = 10^{+15} FLOPS



High-resolution & Robust Algorithms

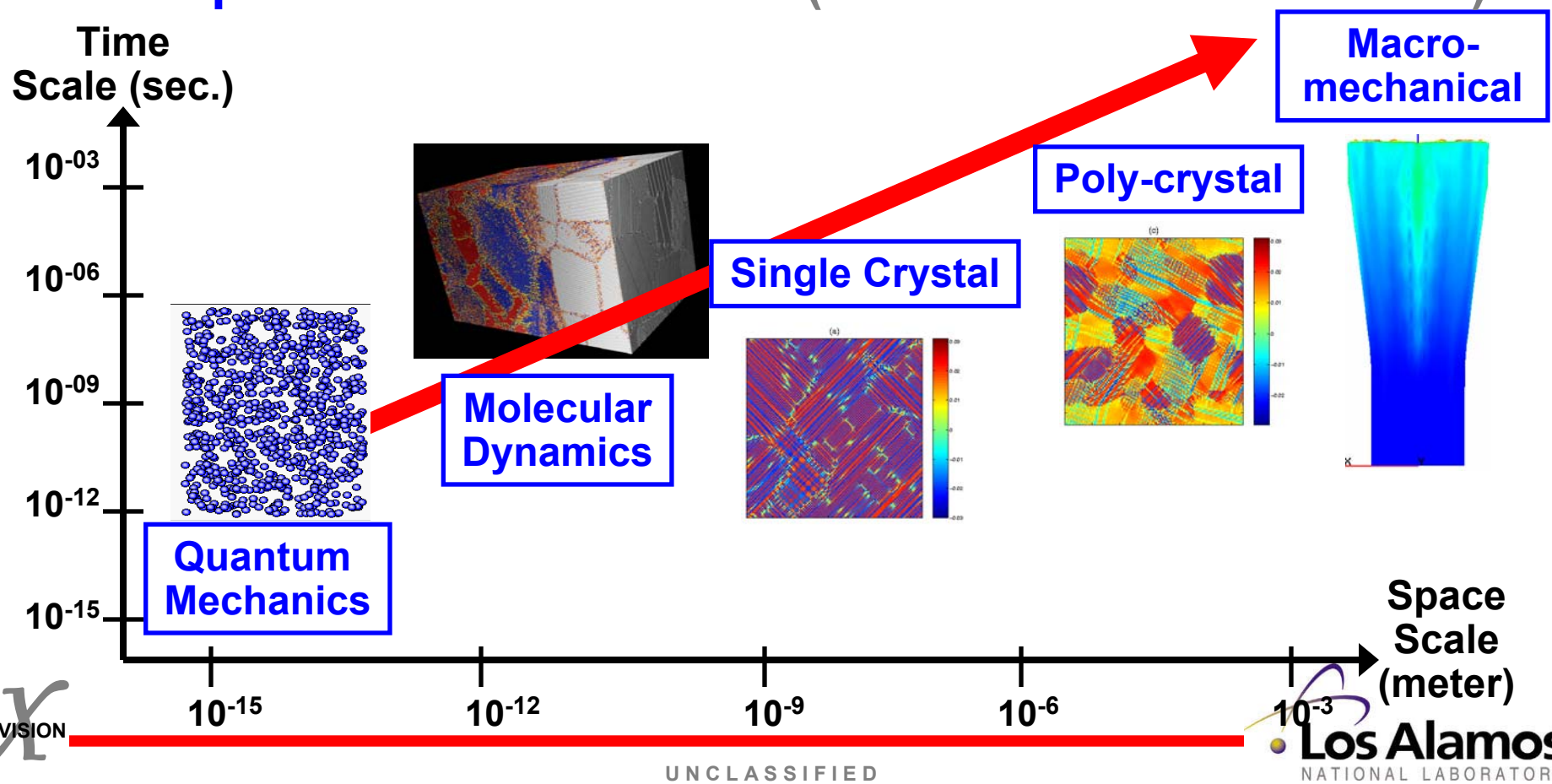
- High-resolution Godunov solvers (Case D) provide up to a factor four improvement in accuracy.



Code-to-code comparisons for the problem of shock acceleration of a diffuse dense gaseous cylinder (Navier-Stokes equations). Reference: Greenough, Rider, and Zoldi, APS-DFD 2001. LA-UR-02-6540, LA-UR-03-0778.

First-principle Physics

- The *first-principle physics* approach to modeling builds the simulation from the bottom-up, starting at the appropriate space-time-energy scales to capture all phenomena of interest (... and their uncertainties).



... And Experimental Measurements!

- Just like there is not statistics without data, there is no Verification and Validation (V&V) without data!

“There are no statistics without data.”

“In statistics, one must always trade-off data for assumptions.”



Michael McKay, LANL

At the SAMO Conference (Santa Fe, NM, 2004)

- In Modeling and Simulation as well ... assumptions are needed to mitigate our lack-of-knowledge (ignorance). V&V also involves trading-off data for assumptions.

Guidance for Structural Dynamics

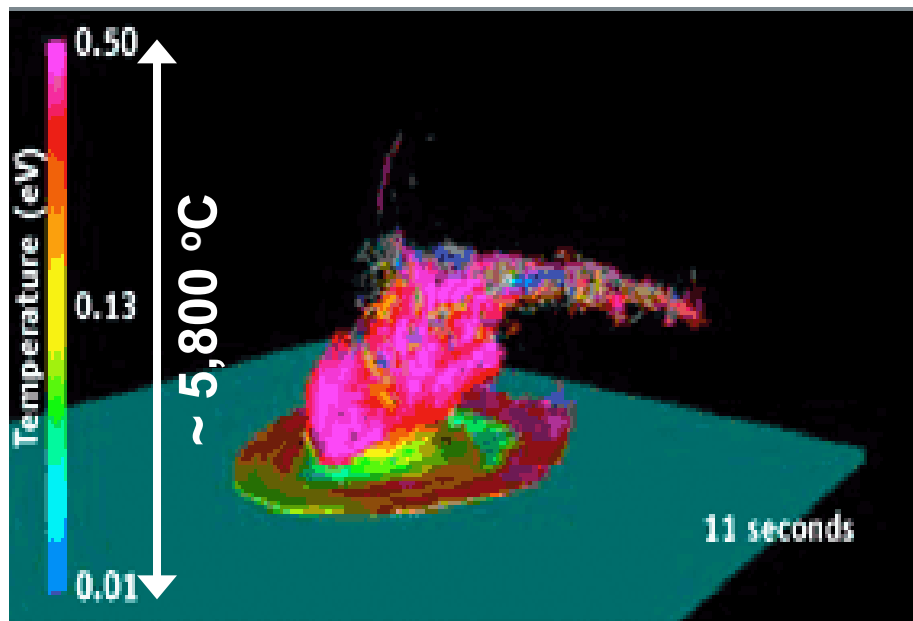
- Represent the geometry with a high degree of fidelity.
- Quantify manufacturing and assembling variability.
- Assess the asymptotic regime of convergence with a mesh refinement; quantify the numerical uncertainty.
- Implement models based on first-principle mechanics or physics to describe the materials, initial conditions, boundary conditions, energy dissipation mechanisms, forcing functions, and external loadings.
- Use appropriate solvers; stay away from low-order approximations such as modal truncation.
- Propagate the sources of uncertainty, variability, and lack-of-knowledge forward through the numerical simulation.

Outline

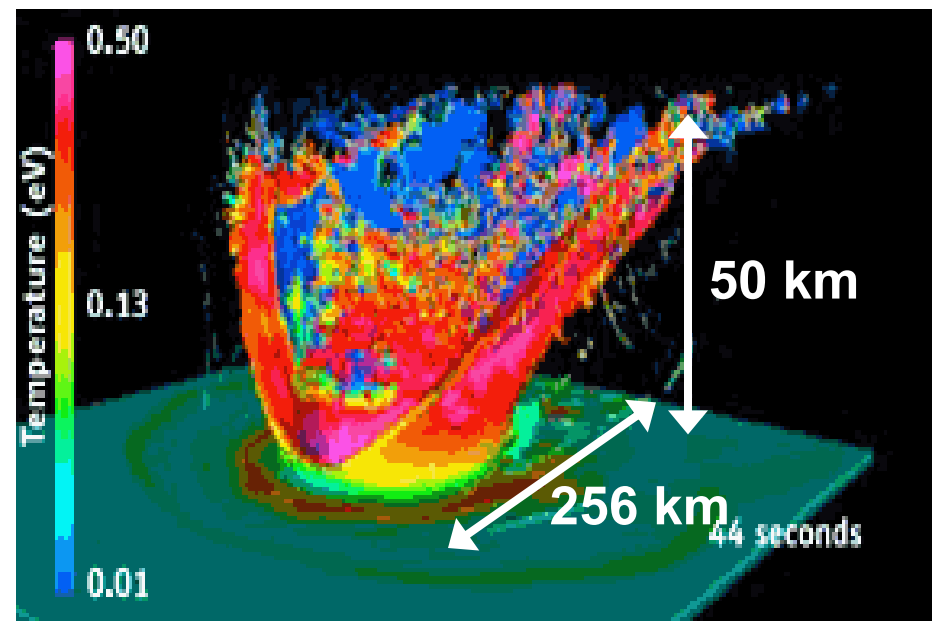
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Simulation of the “*Dinosaur Killer*”

- Pictures illustrate the simulation of a 10-km diameter asteroid impact at Chicxulub, Mexico, believed to have triggered the extinction of dinosaurs.^(#)



Time = 11 seconds



Time = 44 seconds

(#) Credit: G. Gislser, LANL. Shown are density iso-surfaces colored by the temperature of materials, in units of eV.

“*Validation*” of Impact Simulations

- This example poses interesting questions in terms of validation ... Test measurements are severely lacking!
- The only “*hard data*” are inferences of the radiation fluence ($\sim 5\text{-to-}10 \text{ calories.cm}^{-2}$) from measurements of South-facing surfaces of fossilized trees in Colorado, more than 2,000 km away from Chicxulub, Mexico.
- The equations-of-state and opacities of materials are obtained from experiments performed on samples collected in Mexico and the atmosphere. (But where is the estimation of environmental variability?)
- The diameter of the asteroid is calibrated to the size of the crater found off the Yucatan peninsula. (This is to input the “*right*” amount of kinetic energy.)

Typical Steps of Model Validation

- Code verification activities
- Response feature extraction
- Asymptotic convergence of discrete solutions
- Local sensitivity study (finite difference-based)
- Design of computer experiments
- Global sensitivity (variance-based), effect screening
- Development of fast-running meta-models
- Uncertainty propagation and assessment
- Test-analysis comparison and correlation
- Model revision and parameter calibration
- Extrapolation of prediction accuracy and uncertainty

Feed-back?



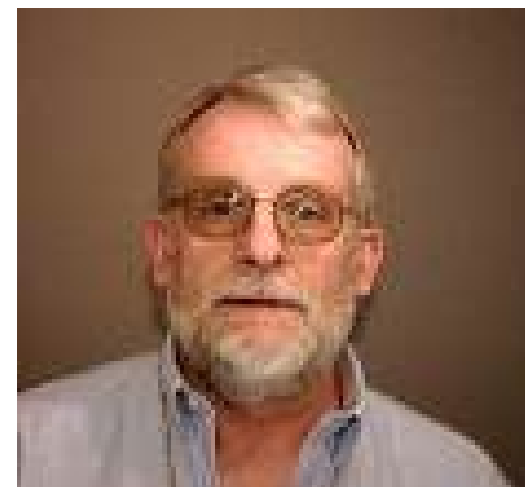
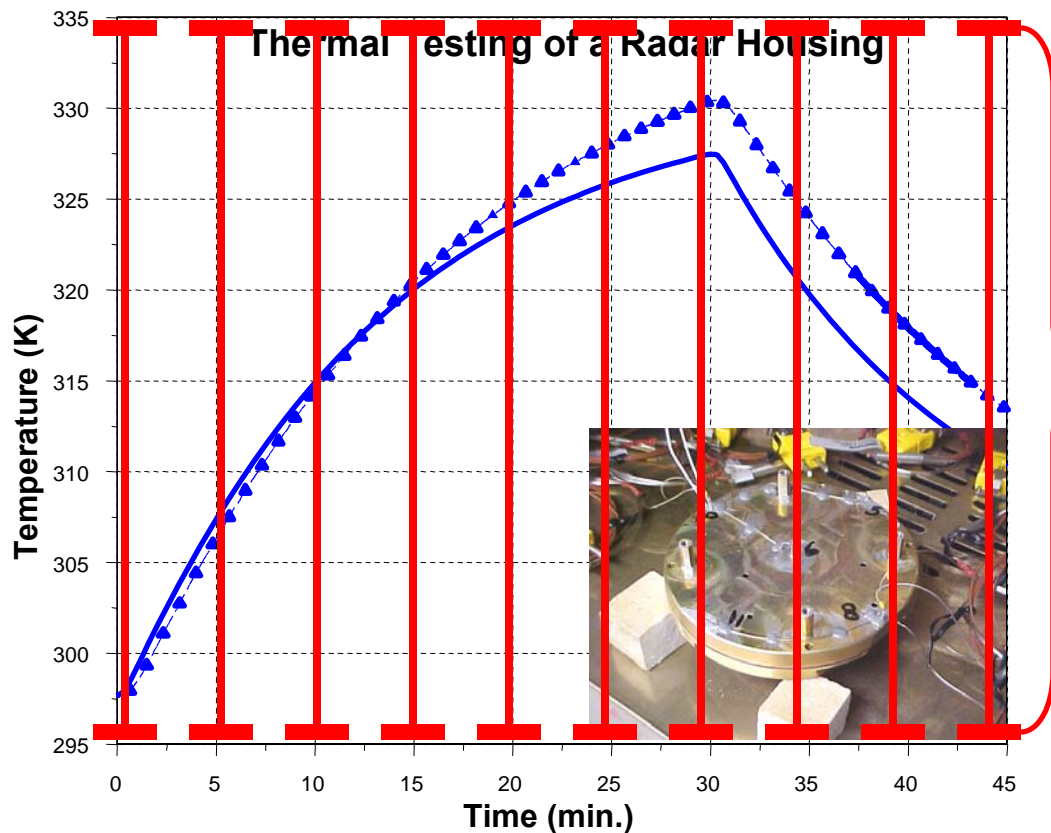
Lessons Learned

- The measurement uncertainty bounds must *always* be quantified when analyzing test data.
- Likewise the uncertainty bounds of discrete solutions must *always* be quantified when running codes.
- The sources of uncertainty in the problem must be assessed, propagated through the simulation, and the resulting uncertainty of predictions must be quantified ... *All of it*, not just uncertainty due to variability.
- If assumptions are formulated in the process of performing these tasks above, then the *robustness* of codes and their predictions should be demonstrated.

 This is what it takes to achieve *confidence*!

Lesson #1

- **Measurements without experimental error bounds are meaningless.** (Replicates, replicates, replicates ...)



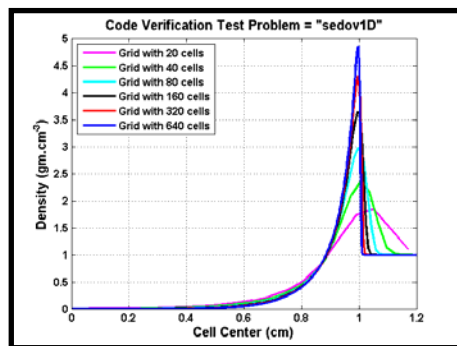
Tim Trucano

V&V Pioneer at Sandia National Laboratories, New Mexico

(Reference: Tim Trucano, "V&V Principles and Challenges," 2006 Nuclear Explosives Code Developers Conference (NECDC|06), Los Alamos National Laboratory, Los Alamos, New Mexico, October 23-27, 2006.)

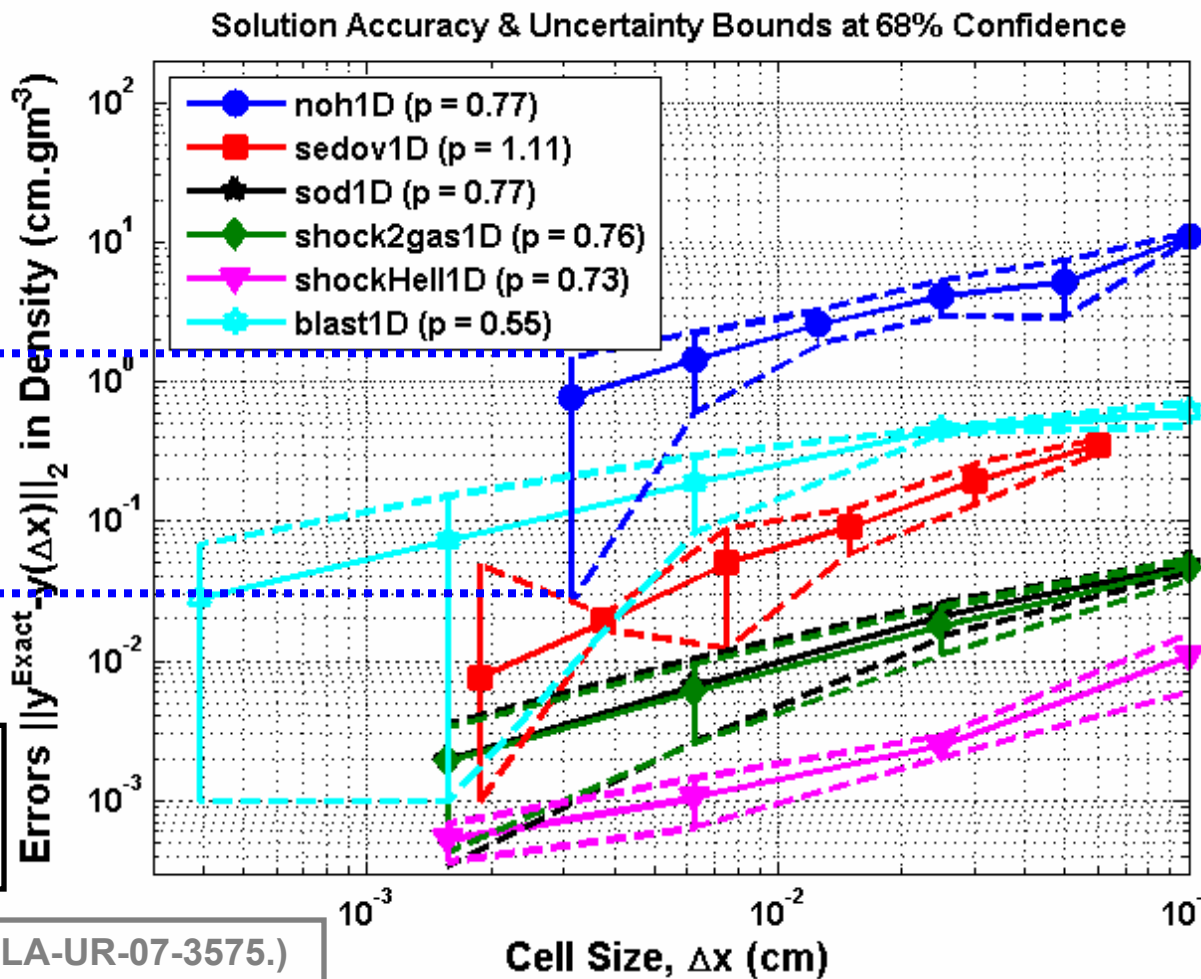
Lesson #2

- Predictions without numerical uncertainty bounds are meaningless. (Do your mesh-refinement homework!)



Bounds of Numerical Uncertainty

Uncertainty bounds from 12,256 runs of six hydrodynamics test problems.



(Pictures extracted from LA-UR-07-3575.)

Lessons #3–4

- One should strive to quantify all uncertainty in the problem, no matter where it comes from, no matter what its nature is.



Jane Booker

BookerScientific, Inc.

*“Combine all you know and determine **how well** you know it.”*

UQ provides the *“how well”* side of the equation.

Assumption 1 | Assumption 2 | ... | Assumption N

Key = Understand the extent to which predictions and uncertainties are sensitive (or *robust*) to assumptions.

Uncertainty in Structural Dynamics

- Lack of control over the environmental variability and test settings: temperature, humidity, materials, inputs.
- Errors made during testing: calibration, measurement errors, aliasing, leakage, etc. Test repeatability: unit-to-unit, operator-to-operator, test-to-test variability.
- Tolerance, manufacturing, and assembling variability.
- Uncertainty about loads, boundary conditions, initial conditions, materials, friction, coefficients of energy restitution, etc.
- Assumptions made during physical testing, such as stationarity, linearity, reciprocity. Assumptions made during modeling such as geometry, material models, types of finite elements, solution algorithms, etc.

Outline

- What does it mean to be predictive?
- Elements necessary to achieve “*predictability*”
- A few lessons learned (as always the hard way ...)
- **An application to the validation of composite models**
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Context

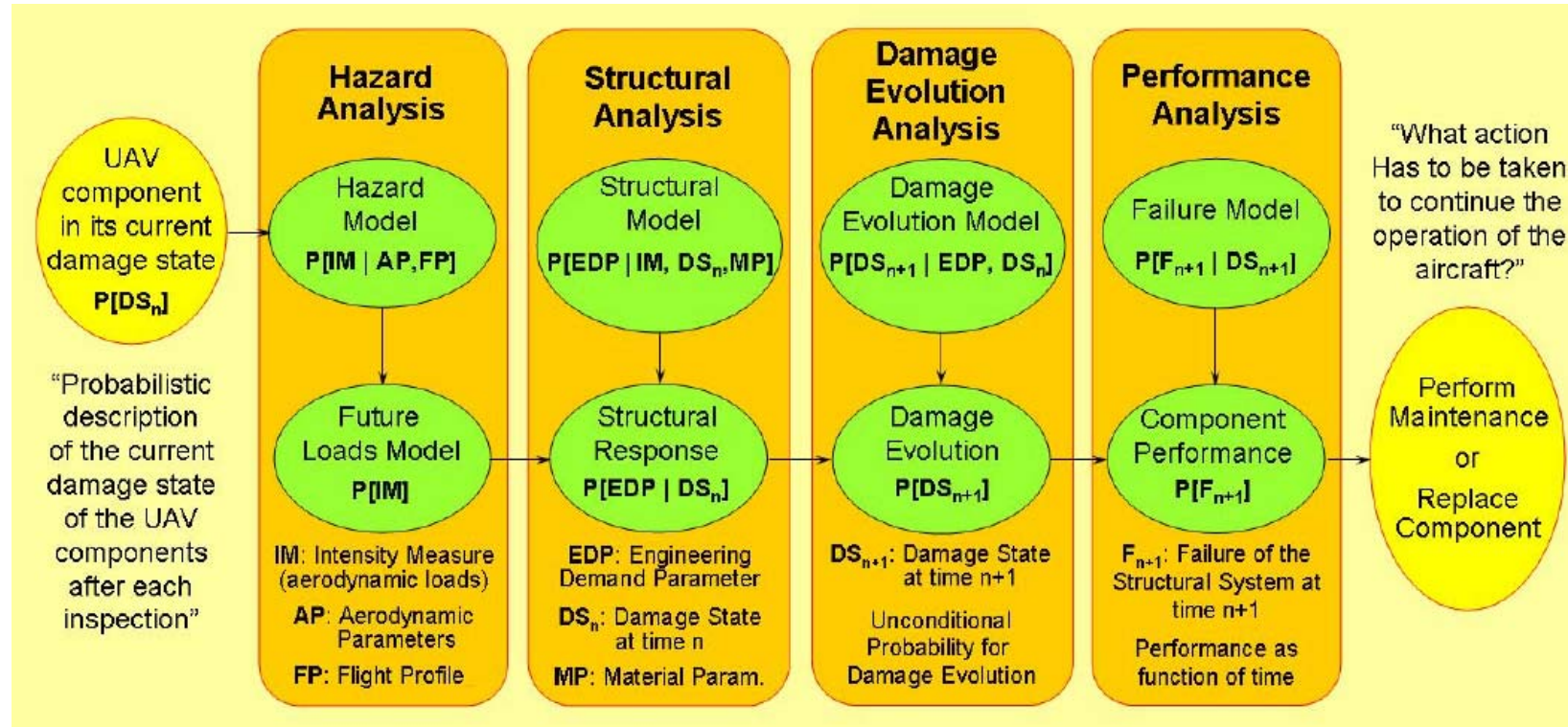
- The context of this work is the development of a predictive capability to simulate damage growth in composite structures and support the deployment of Damage Prognosis solutions on real hardware.



General Atomics Predator Unmanned Aerial Vehicle (UAV)

Damage Prognosis

- The goal of Damage Prognosis is to estimate, in near-real time, the remaining useful life or performance of a structure given its current health/damage state and future mission/loading profiles.

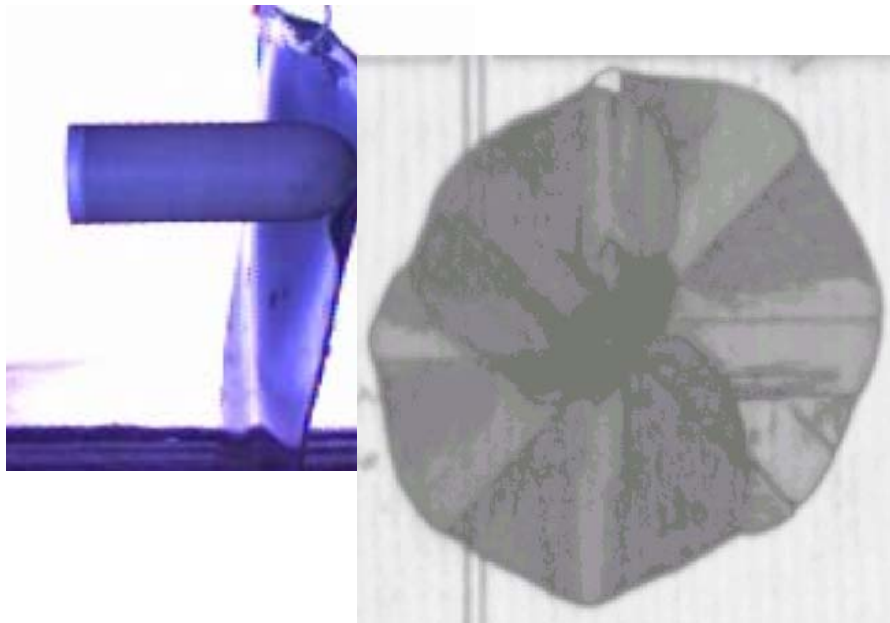


Courtesy of Maurizio Gobbato and Professor Joel P. Conté, UCSD.

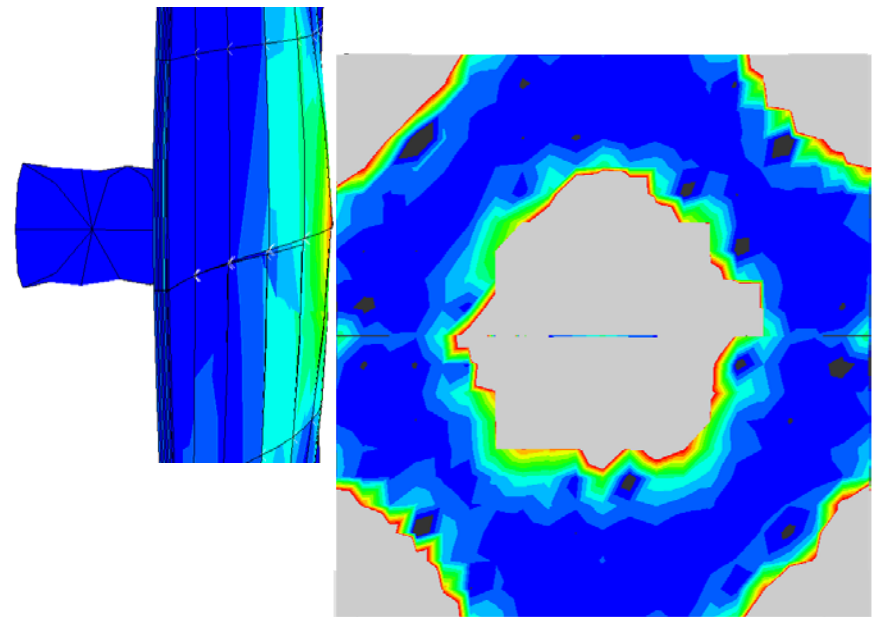
Prediction of Delamination

- This application validates our ability to simulate fiber splitting and delamination that result from impacting multi-layered composite plates with a projectile.

Projectile Impact Experiments and Ultrasound Measurements of Delamination



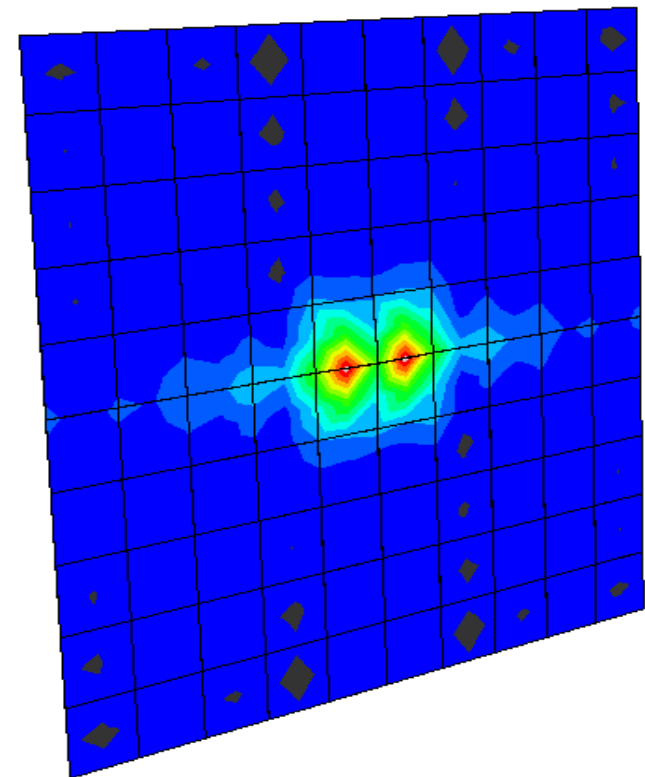
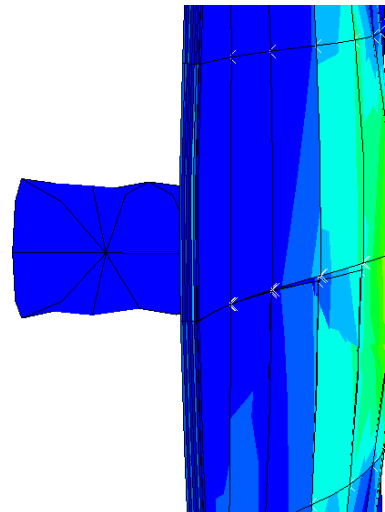
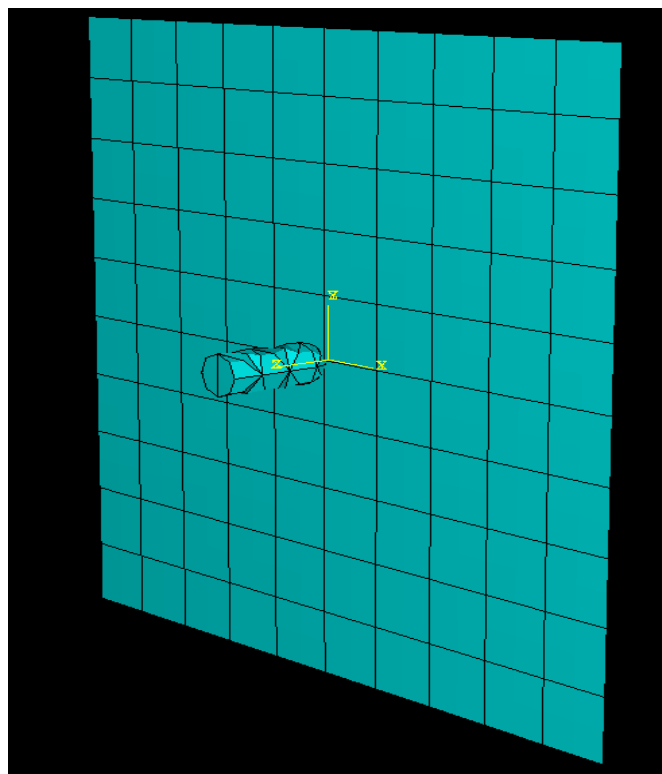
Projectile Impact Simulations and Values of the Delamination Parameter, $0 \leq \lambda \leq 1$



(Reference: Lucero, J.L., Hemez, F.M., Ross, T., Hundhausen, J., Kline, K., Tippetts, T.B., "Uncertainty Quantification of Composite Laminate Damage with the Generalized Information Theory," *Los Alamos National Laboratory LA-14283*, Los Alamos, New Mexico, May 2006.)

Modeling and Simulation (M&S)

- Numerical simulations can be developed to make the predictions of delamination damage and growth, but to what extent are they *credible*?



List of Modeling Assumptions

- Finite element discretization of each ply.
- Linear and orthotropic ply material.
- Contact between projectile and plate is handled via a non-linear (but single-node) Hertz contact model.
- Coupling of damage modes restricted to ply splitting and delamination. (No breakage implemented.)
- Damage is handled via Cohesive Zone Models (CZM).
- No thermal-mechanical coupling.
- Discretization (size of finite elements) must allow fast enough turn-around times of simulation runs.

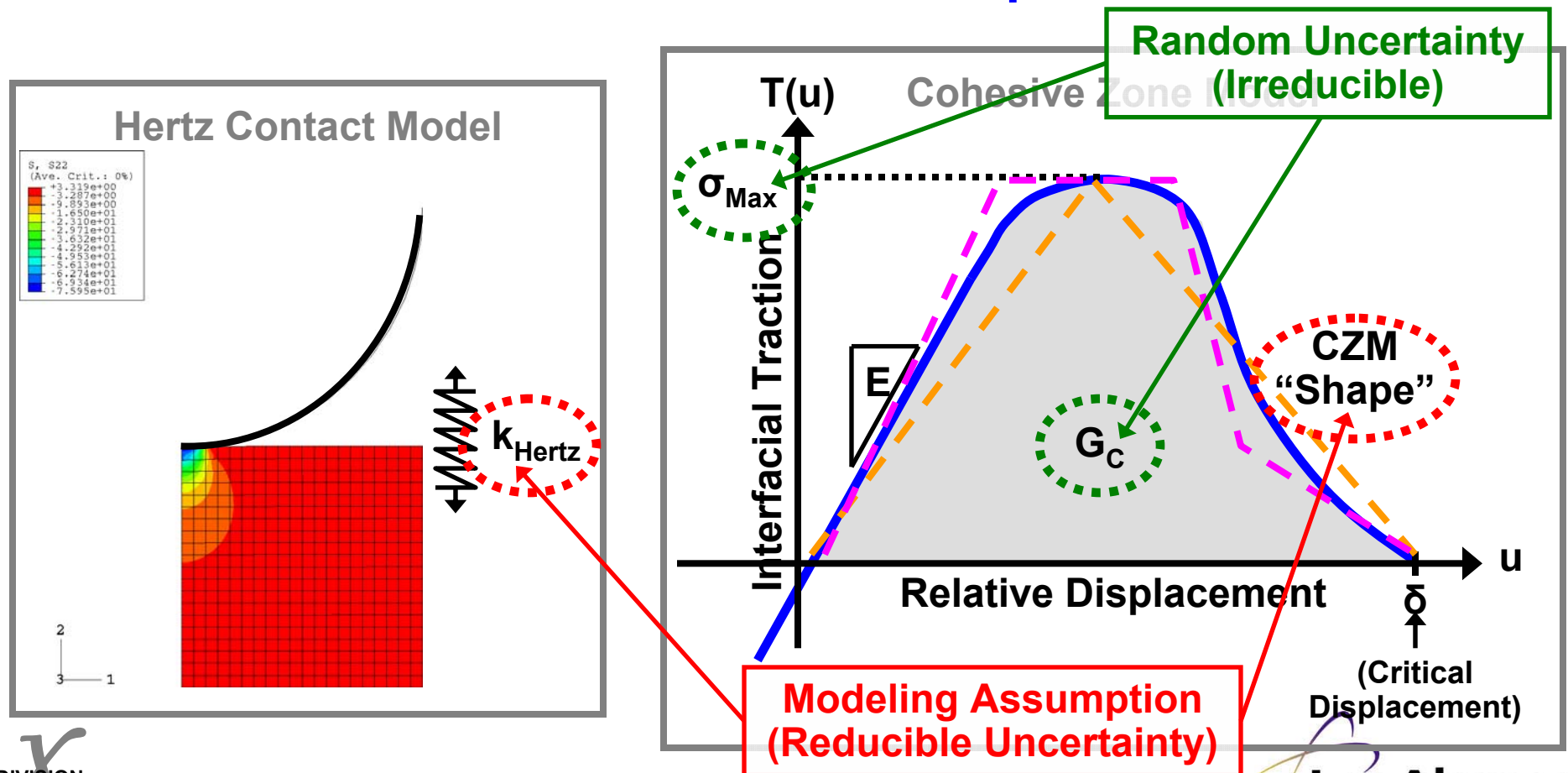
Sources of Uncertainty

- The modeling assumptions translates into a list of parameters or flags that can be exercised during the numerical simulations of plate vibration and impact.

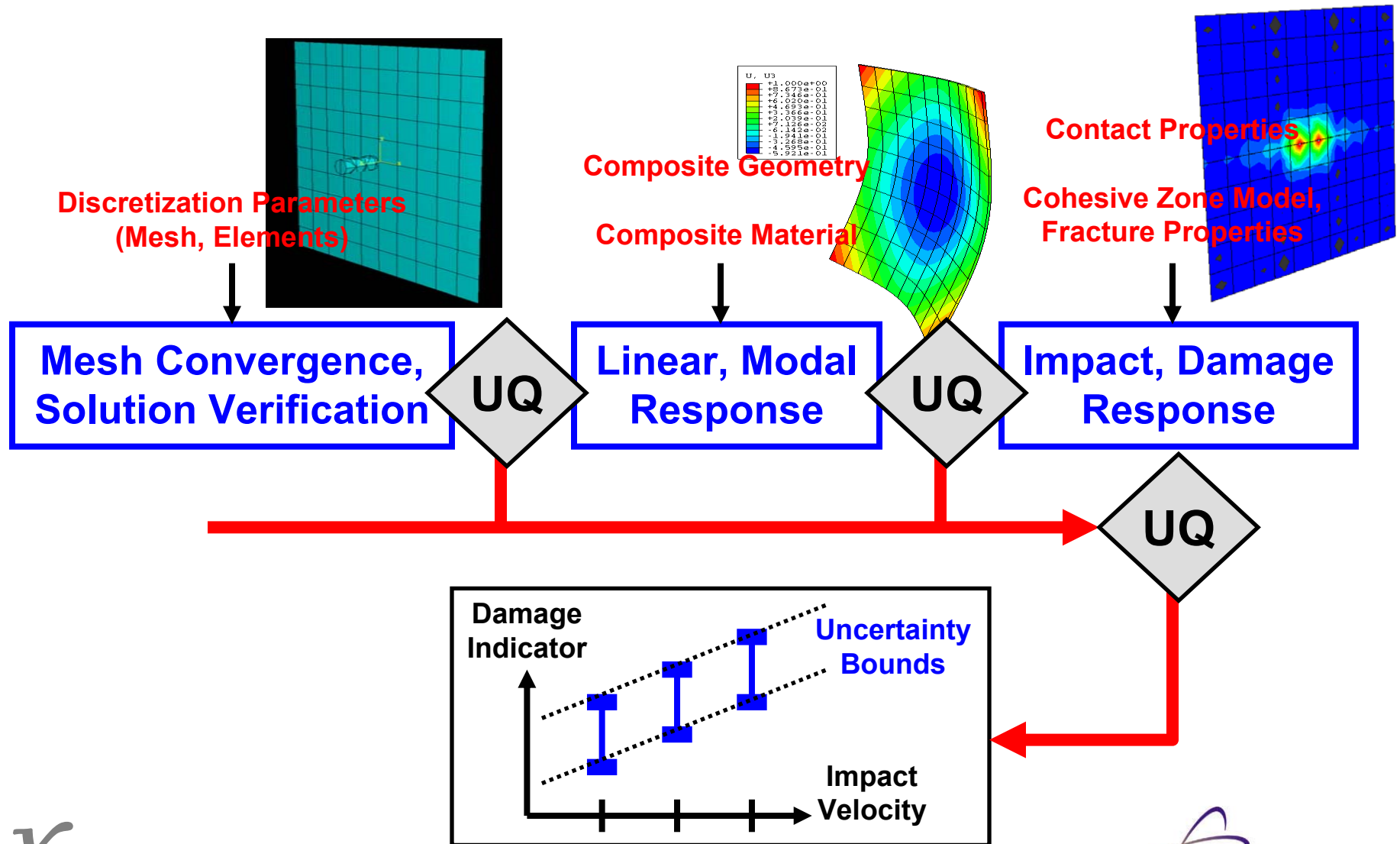
Source	Description	Type
Ply orientation angles	$\theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6, \theta_7, \theta_8$	Variability
Composite material	$E_{11}, E_{22}, E_{33}, G_{12}, G_{13}, G_{23}, E_{12}, E_{13}, E_{23}, \rho$	Variability
Fracture properties	$(G_C^{(k)}; T_{Max}^{(k)})$ for each fracture mode ($k = I, II, III$)	Variability
Cohesive Zone Model	Location of CZM finite elements	Assumption
Cohesive Zone Model	Shape of the force-displacement curve	Assumption
Impact velocity	V_I	Variability
Projectile contact	Coefficient of the Hertz contact model, k_{NL}	Assumption
Projectile contact	Shape of the contact model	Assumption
Prediction of fracture	Fracture parameter, $\lambda_F \in [0; 1]$	Fuzziness

Examples of Assumptions

- Simulation uncertainty originates from assumptions made while implementing, for example, the contact and Cohesive Zone Model of composite behavior.



V&V Strategy ... “Divide and Conquer”



Step 1 — Code Verification

- Code verification activities make sure that aspects of the code that matter for the simulation are bug-free.

Frequencies for a Square, Free-free, Isotropic Plate							
Mode (i, j)	(2, 2)	(1, 3)	(3, 1)	(3, 2)	(2, 3)	(4, 1)	(1, 4)
Analytical	13.49	19.79	24.43	35.02	35.02	61.53	61.53
HKS/Abaqus™	13.48	19.69	24.45	34.95	34.95	62.45	62.45
Error (%)	0.03	0.53	-0.05	0.20	0.20	-1.50	-1.50

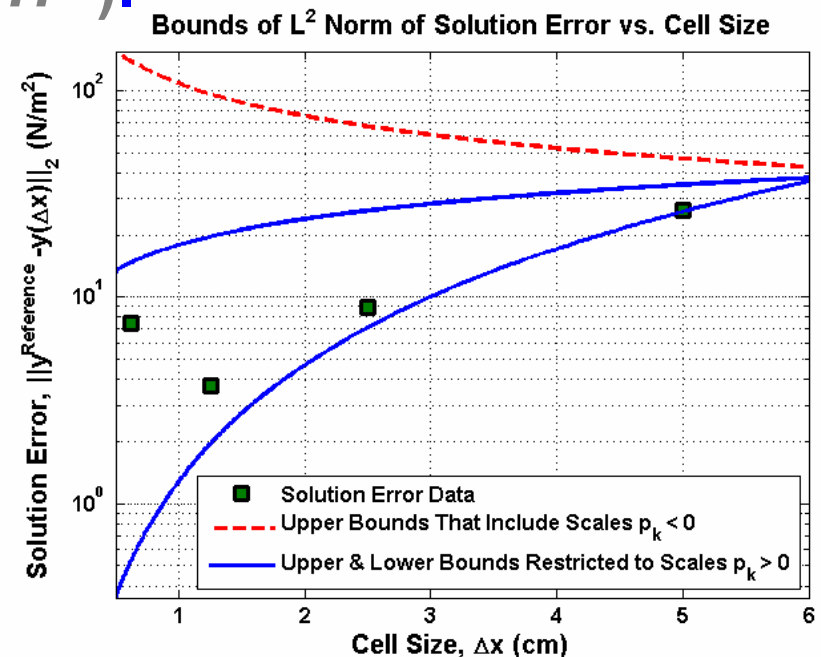
Frequencies for a 3-ply, Simply Supported, Orthotropic Plate				
Stiffness ratio E_{x1}/E_{x2}	Density ratio ρ_1/ρ_2	Analytical	HKS/Abaqus™	Error (%)
10	1	0.098	0.098	-0.026
15	1	0.112	0.112	-0.016
15	3	0.095	0.095	-0.015

Step 2 — Solution Verification

- Solution verification activities assess the asymptotic convergence of discrete solutions (“what element size Δx should be used to run the problem?”) and quantify the level of numerical uncertainty (“what are the error bounds around the solution?”).

Solution Verification of Modal Response		
Mode Number	Convergence Rate	Grid Convergence Index
1	$p = 0.82$	GCI = 0.91%
2	$p = 2.17$	GCI = 0.31%
3	$p = 1.47$	GCI = 0.78%
4	$p = 2.82$	GCI = 0.15%
5	$p = 1.70$	GCI = 0.61%

(Legend: Theoretical rate is $p^{\text{Theory}} = 2$.)



Bounds of Solution Uncertainty for the Hertz Contact Problem

(References: Left: LA-UR-05-0569; Right: LA-UR-06-8884.)

Step 3 — Material Testing

- Each plate is 152.0 mm (6.0 inch) square, 1.0 mm (0.04 inch) thick, and made of eight orthotropic carbon fiber plies. Each ply is 0.127 mm (0.005 inch) thick. The ply orientation from top to bottom is [0; 45; 90; -45; -45; 90; 45; 0] degrees.

Symbol	Mean (μ)	Standard Deviation (σ)
E_{11}	$132.4 \times 10^9 \text{ N/m}^2$	3% of mean
E_{22}	$9.1 \times 10^9 \text{ N/m}^2$	2% of mean
G_{12}	$4.5 \times 10^9 \text{ N/m}^2$	3.6% of mean
ν_{12}	0.30	Unknown
ν_{23}	0.40	Unknown
ρ	$1,522.0 \text{ kg/m}^3$	2.5% of mean



Step 4 — Effect Screening

Factor	Symbol	Definition
1	θ_1	Ply angle 1 (top-most layer of fibers)
2	θ_2	Ply angle 2
3	θ_3	Ply angle 3
4	θ_4	Ply angle 4
5	θ_5	Ply angle 5
6	θ_6	Ply angle 6
7	θ_7	Ply angle 7
8	θ_8	Ply angle 8 (bottom-most layer of fibers)
9	E_{11}	Modulus of elasticity in the fiber direction (1-fiber)
10	E_{22}	Modulus of elasticity in the transverse direction (2 transverse)
11	G_{12}	Shear modulus in the plane (1-fiber, 2-transverse)
12	ν_{12}	Poisson's ratio in the plane (1 fiber; 2 transverse)
13	ν_{23}	Poisson's ratio in the plane (2-transverse; 3-out-of-plane)
14	ρ	Material density
15	M_a	Mass added by an accelerometer and its cabling

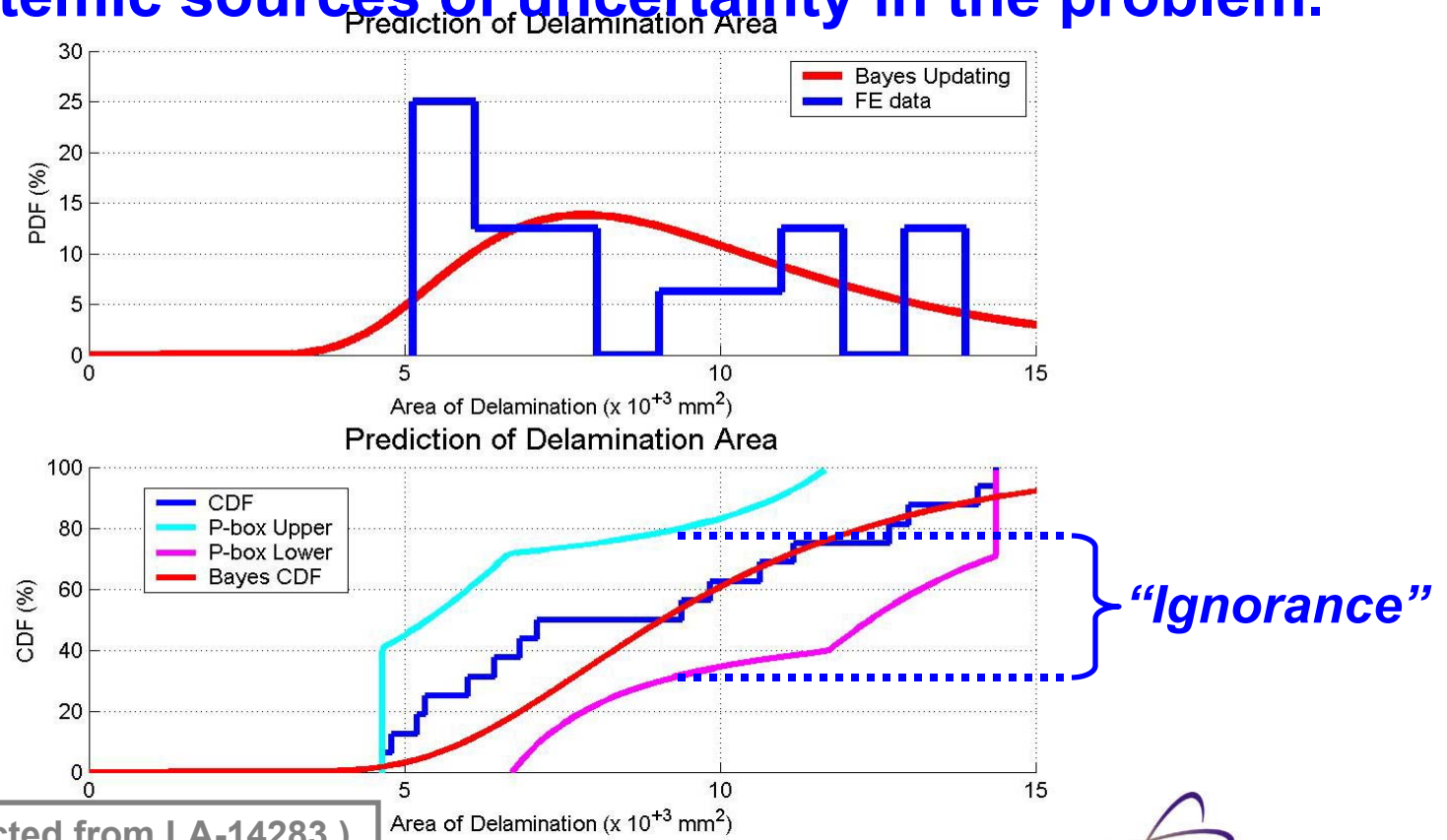
Step 5 — Uncertainty Propagation

Definition of Main Sources of Uncertainty for Impact Simulations			
Symbol	Description	Range	Reducible?
CMZ	Shape of the Cohesive Zone Model (CZM) of damage evolution	A or B or C [Unitless]	Yes
k_{Hertz}	Stiffness of the Hertz contact model between the projectile and plate	A or B [Unitless]	Yes
σ_{Max}	Maximum stress that the fiber can withstand before fracture appears	$34\text{--}43 \times 10^{+6}$ [N.m ⁻²]	No
G_c	Total energy that the fiber can store before being fully separated	200–590 [J.m ⁻²]	No

Legend	
Epistemic	Due to our particular choices of modeling assumptions. (Can be reduced through modeling and testing.)
Randomness	Due to variability, non-uniformity of manufacturing and curing processes. (May be more accurately characterized, but cannot be reduced.)

Step 6 — Prediction + Uncertainty

- The area of delamination due to projectile impact is predicted, together with its bounds of uncertainty. The quantification illustrated below is not probabilistic due to epistemic sources of uncertainty in the problem.



(Picture extracted from LA-14283.)

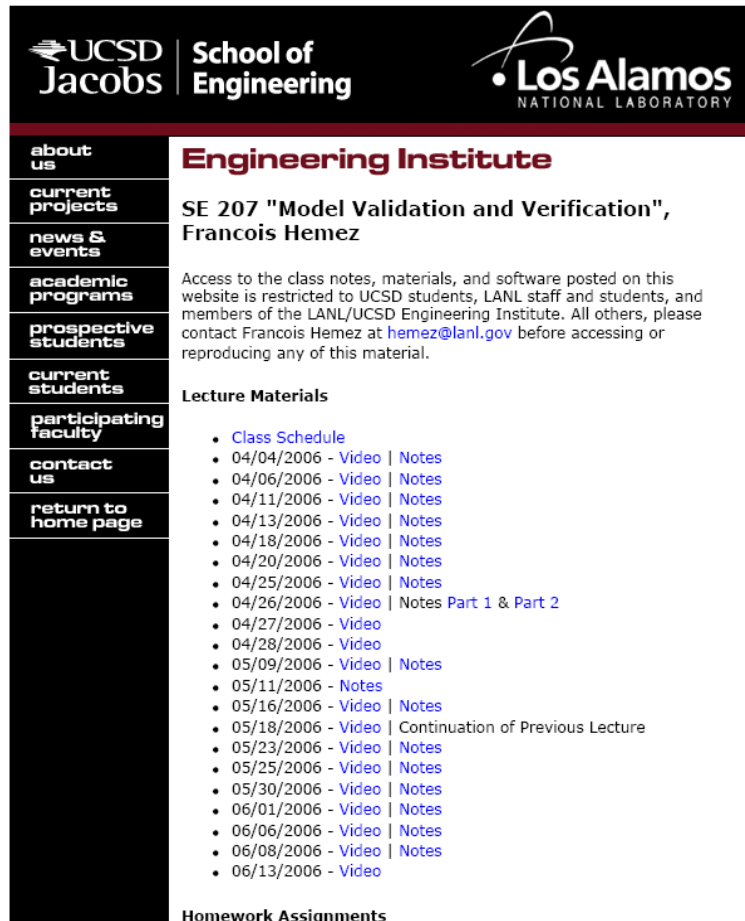
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The Educational Component

- A formal V&V Program cannot be successful without a strong commitment to training and education.

EEL - Engineering Education Initiative



The screenshot shows a website for the Engineering Institute, a partnership between UCSD Jacobs School of Engineering and Los Alamos National Laboratory. The page title is "Engineering Institute". A navigation menu on the left includes links for "about us", "current projects", "news & events", "academic programs", "prospective students", "current students", "participating faculty", "contact us", and "return to home page". The main content area is titled "SE 207 'Model Validation and Verification', Francois Hemez" and includes a disclaimer about access to class notes and software. Below this, there is a "Lecture Materials" section with a list of dates and links to "Video" and "Notes" for various dates from 04/04/2006 to 06/13/2006. At the bottom, there is a "Homework Assignments" section.

- In partnership with the University of California San Diego (UCSD), LANL is developing a formal degree in *“validated simulations.”*
- A graduate-level course on V&V was offered at UCSD during the Spring 2006 (first time in a U.S. University).
- V&V is an integral part of the Los Alamos Dynamics Summer School, that graduated 125 students so far.
- We have also developed a two-day short course for internal training and collaboration with industry.

... Don't Turn to the "Dark Side"

"Luke, join me and together we will crush these rebellious scientists who think that V&V can be useful!"

Questions?

*"Calibration!
Calibration!"*