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Stochastic simulation and uncertainty quantification at Sandia National Labs

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NAFEMS Stochastic Working Group

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Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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Background

Sandia National Laboratories

- Mission: Design and qualify engineering components and systems for US Department of Defense
- Engineering Sciences Center
  - Provides technical basis
  - Perform testing and modeling/simulation
- My org: Uncertainty quantification (UQ), verification & validation (V&V), and credibility processes
- Question for today:
  - What is the role of uncertainty analysis, stochastic modeling, and validation?

The role of tests

- Provide evidence for design and qualification
- “Real world” observations
- Limited in number and control of environment

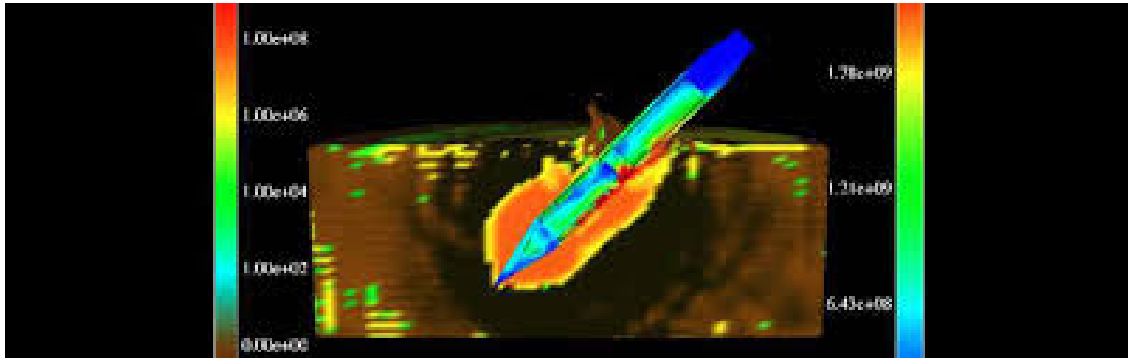
Thermal testing

Rocket sled

Images from sandia.gov

The role of modeling/simulation

- Complements testing - can simulate before building
- Good control over environment
- Number of observations much higher
- Not “real world”



- What questions can we answer with testing, M&S?
- Specifically, what does stochastic simulation add?

Images from sandia.gov

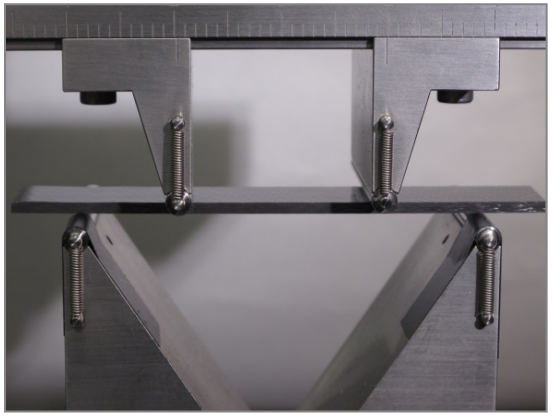
What is stochastic simulation?

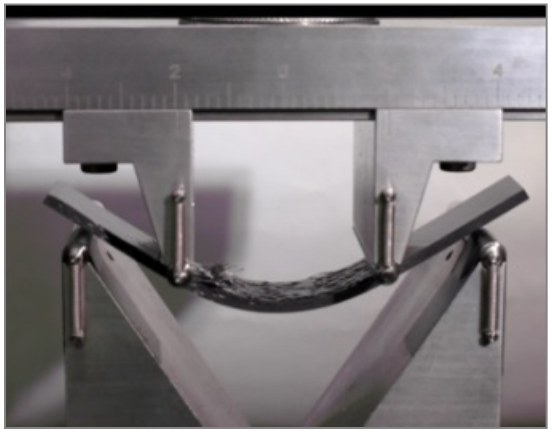
Sandia examples:

1. Uncertainty quantification of a laminate composite
2. Multiscale modeling for solid mechanics
3. Design of a shaped charge
4. Validation of a foam model

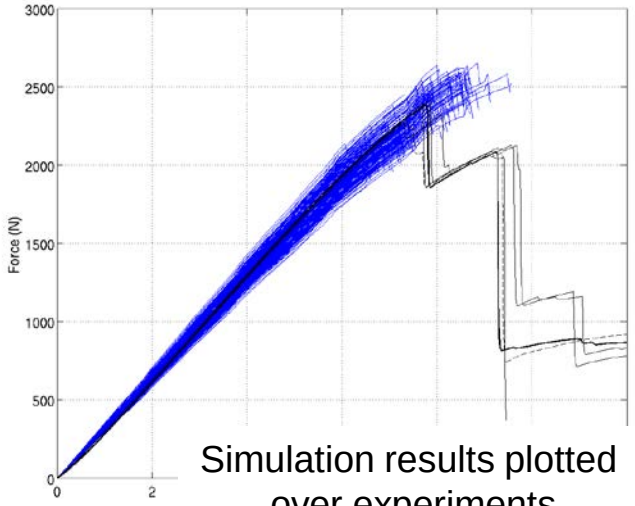
1. UQ of a laminate composite

Shawn English. *Uncertainty Quantification in Material Parameter Calibration for Laminate Composite Failure in Flexure*. ASME V&V Symposium 2015.

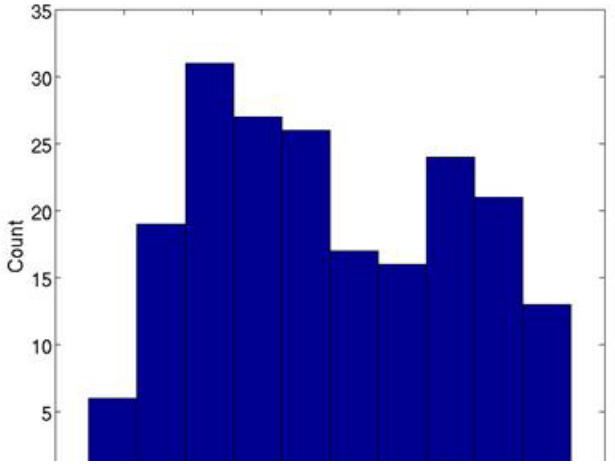




- Model up to first failure
- Compare repeated tests to simulations w/ uncertainty



Simulation results plotted over experiments

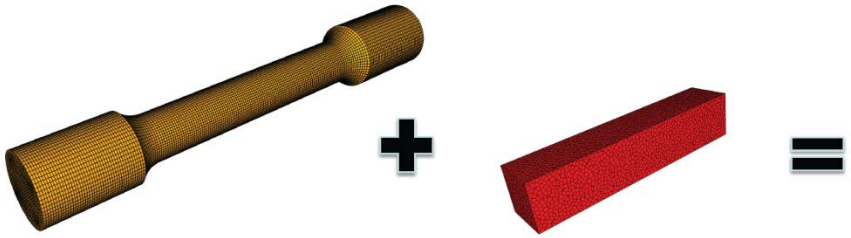


Histogram of simulated peak load

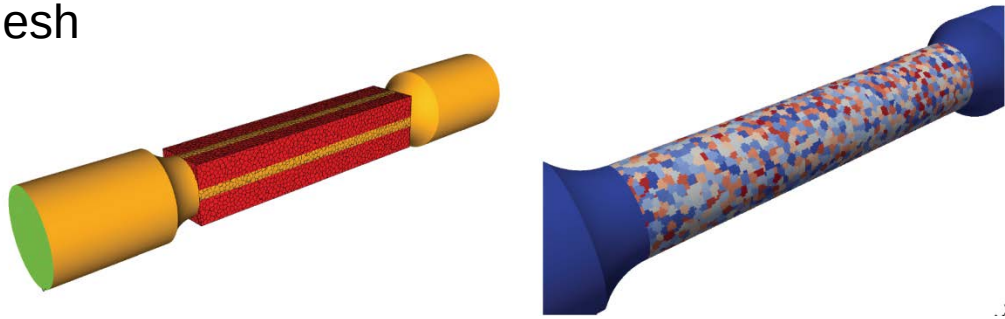
- What are we trying to model?

2. Multiscale modeling for solid mechanics

- We can capture macroscale variability, what about microscale variation within each part?
- How to include microscale material variability in our macroscale simulations?



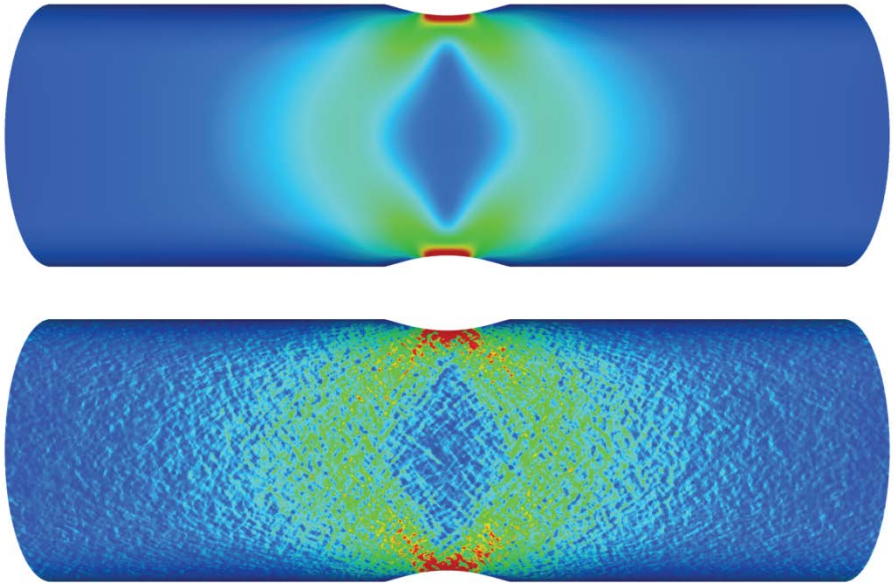
Voronoi Overlay of Hexahedral Mesh



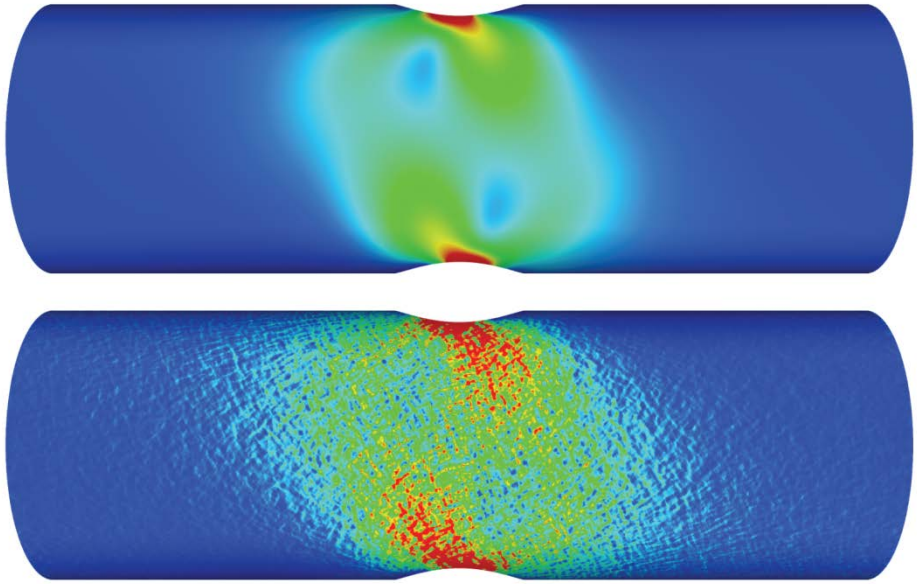
Direct numerical simulations in solid mechanics for understanding the macroscale effects of microscale material variability

Joseph E. Bishop, John M. Emery, Richard V. Field, Christopher R. Weinberger, David J. Littlewood

Continuum vs. microscale modeling



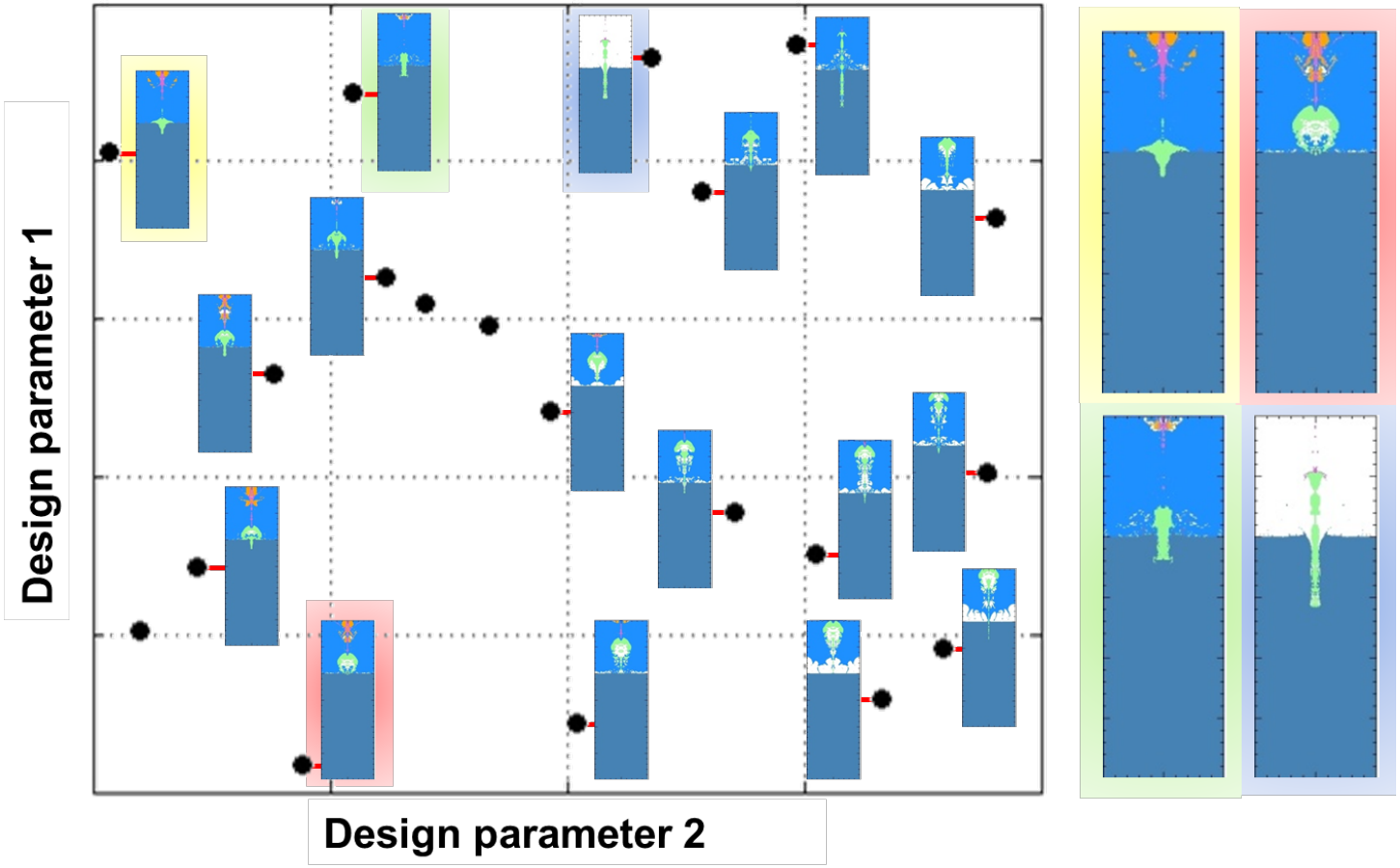
Axial Load



Axial Load + Torsion

- Scope and scale: more detail vs. larger scope
- Hierarchy concept – take advantage of information between models of scale and scope
- Can we test?

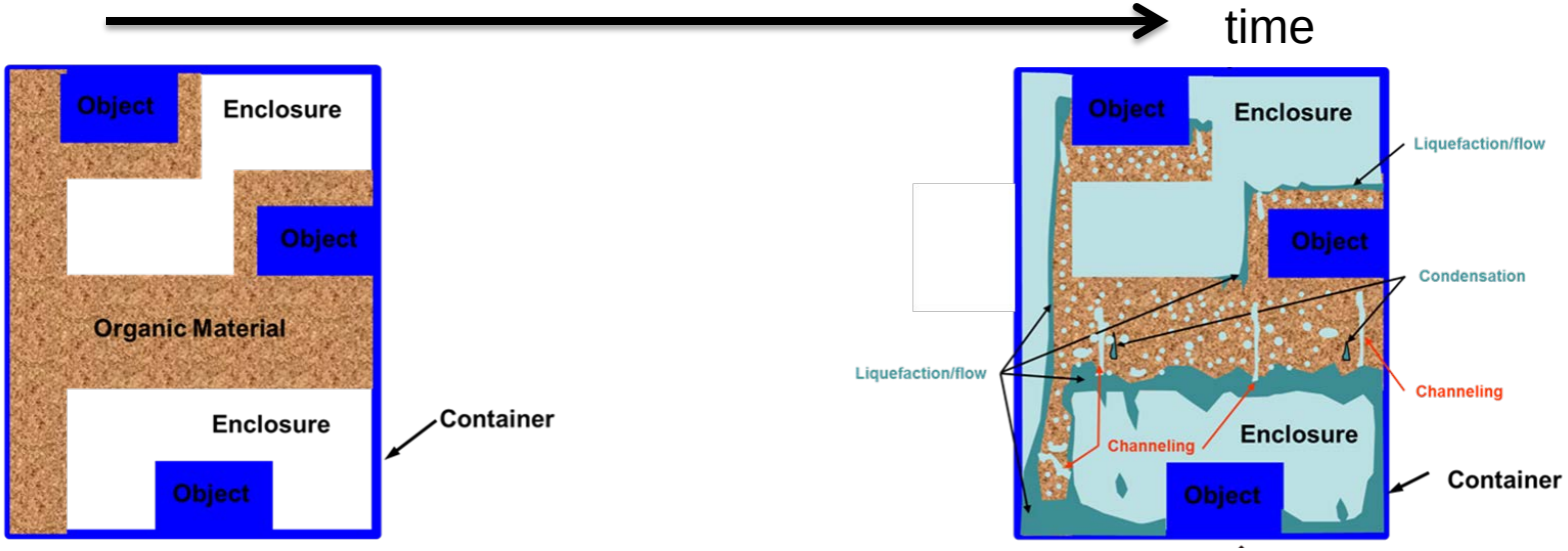
3. Design of shaped charges



- Variability driven by physics – not captured in model
- Account for it in parameters → model form error

4. Foam decomposition analysis

Ryan Keedy, Victor Brunini, Sarah Scott, Amanda Dodd. *Uncertainty Quantification Assessment of Porous Media Modeling of Polyurethane Foam in a Sealed Container*. ASME V&V Symposium 2015.



- ~~How do we know we are right?~~
- Why do we believe in our simulations?

Summary

Sandia examples:

1. Uncertainty quantification of a laminate composite
   - Calibration; Epistemic vs. aleatoric uncertainty
2. Multiscale modeling for solid mechanics
   - Relating models of different scope/scale/fidelity
3. Design of a shaped charge
   - Convolution: model form & parametric uncertainty
4. Validation of a foam model
   - Relate test and simulation – need uncertainty

Guide for Verification and Validation in Computational Solid Mechanics, 2006, ASME. ASME V&V 10-2006.

I didn't mention verification

physics understanding → math models → code solution

Why do simulation?

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- Gain insights into system behavior and response to a variety of environments
  - What questions can we answer with simulations?
- Level of insight is limited by "predictive capability"
  1. The fidelity of the simulation
  2. Uncertainty or variability in the response
  3. Credibility of the work

- Many other ways to frame this issue

Factors of predictive capability

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The fidelity of the simulation

Coarse/ empirical models

High fidelity

Uncertainty or variability in the response

Don't know

Characterized variability and all sources of uncertainty

Credibility of the work

Didn't think about it

Experienced team, documented process, V&V, etc. Peer reviewed.

This is just one idea, see also PCMM.

Factors of predictive capability

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Some of the issues

The fidelity of the simulation

Scale and scope

Uncertainty or variability in the response

Epistemic vs. aleatoric

Model form error vs. parametric uncertainty

Numerical uncertainty

Credibility of the work

Why do we believe?

Uses of the model

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Discovery → Support Decisions → Risk management

vs. what capabilities do we have

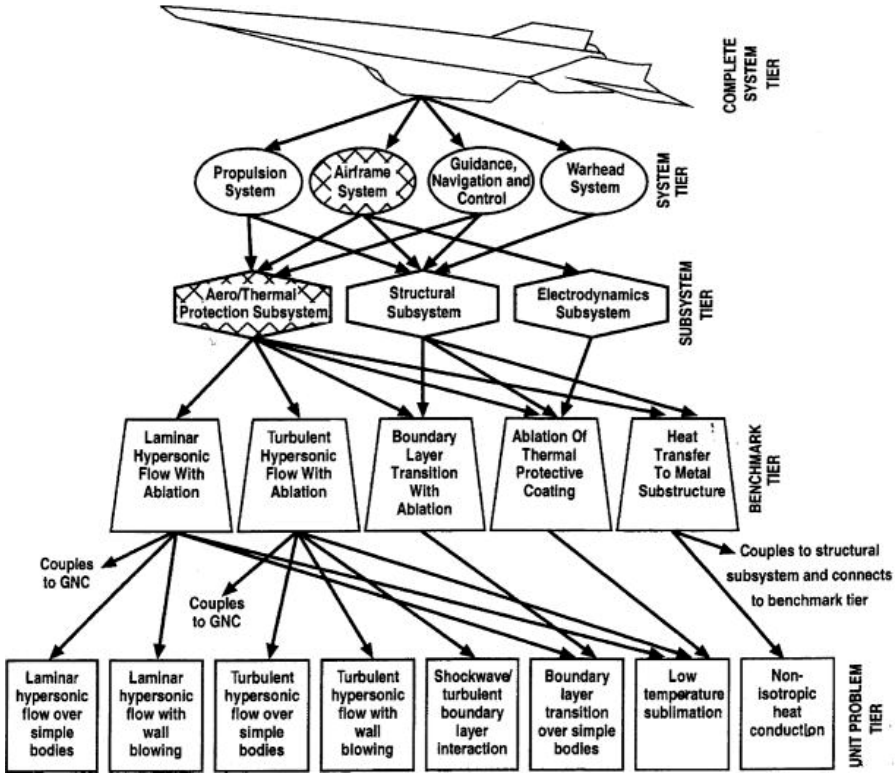
- The fidelity of the simulation
- Uncertainty or variability in the response
- Credibility of the work

and at what cost?

Can we tell a complete story? Often we only see one piece at a time – hard to tell the value.

Hierarchy of test and simulation

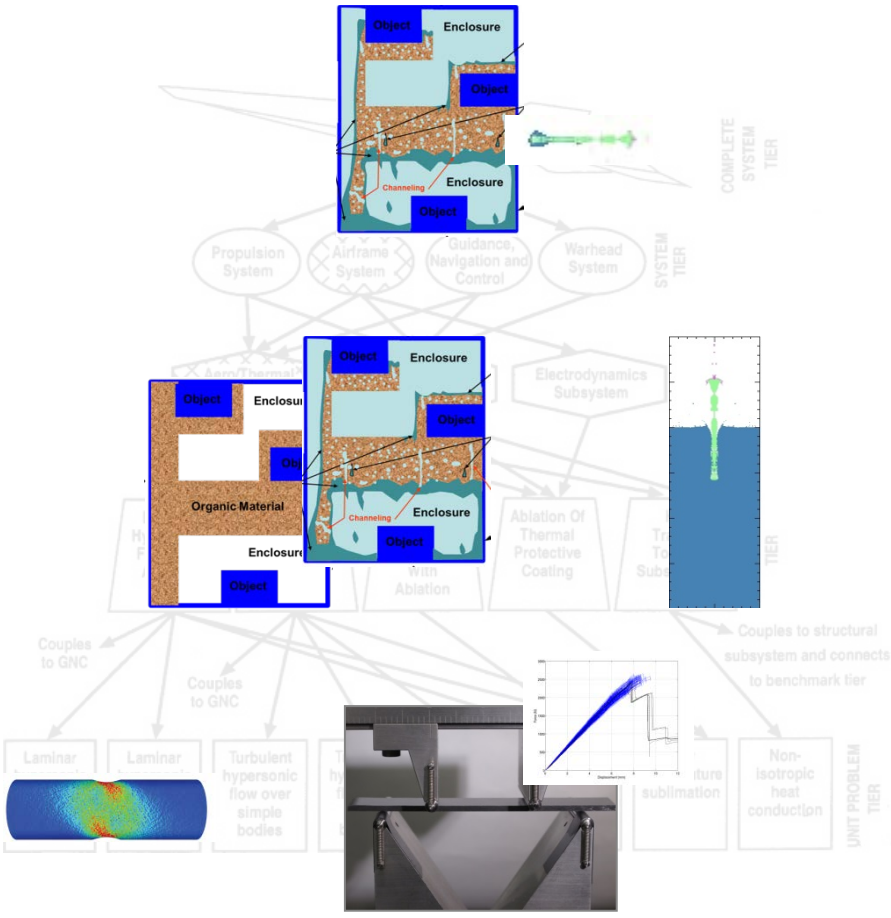
- Arrange tests and sim for the whole project
- Example of axes:
  - System complexity
  - Environment complexity
  - Maturity of hardware design or model



Oberkampf, Trucano, Hirsch. Verification, validation, and predictive capability in computational engineering and physics. *Appl. Mech. Rev* 57(5), 345-384

Hierarchy of test and simulation

- How far across the hierarchy is ___ relevant?
- Made up example…
  - Spatially varying foam
  - Heated → decomposes
  - Pressurized component
  - Want controlled vent
  - Breach the laminate composite wall w/o damaging ___ inside
- Do stochastic events drive the story?



Cost/benefit

- Stochastic modeling adds information
- Design & qualification may not NEED this level of insight
- Design for stochastic behavior, or worst case scenario?
- Need modeling, uncertainty, AND credibility
  - Lot of talk about modeling effort + computational cost
- Credibility is EXPENSIVE – especially for stochastic sim.
  - Can we get the data?
  - Identify &characterize input uncertainty?
  - Are we accurate? Does uncertainty match?
- Balance attention on known vs. unknown unknowns

Stochastic simulation @ Sandia

Sandia National Laboratories

- Unique mission, HUGE resources, no competition
- Big effort on UQ methods and application, and V&V
- Capability – appropriate for the questions being asked
- Need – does variability/uncertainty drive the story?
- Risk of assuming vs. the cost of knowing
  - Project risk (requirements) and model "use risk"
- Risk management – payoff is unknown,
- **Need more experience**

Thanks

Sandia National Laboratories

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