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Proposal for FY14 V&V Challenge Workshop

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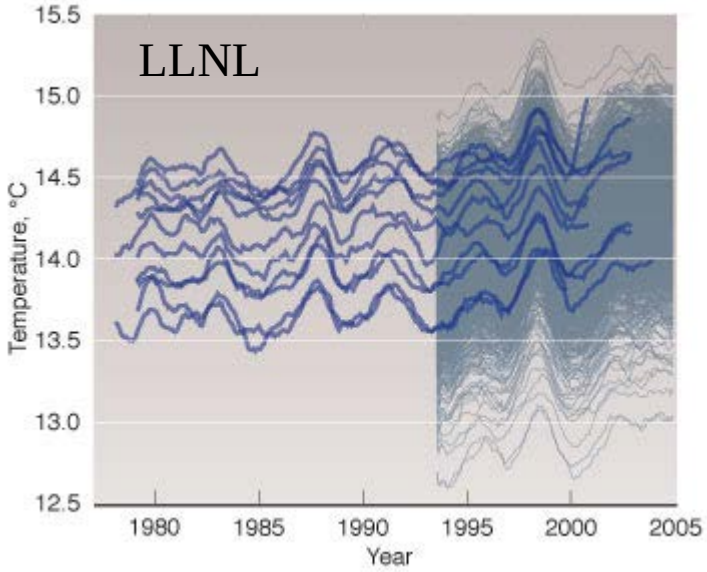
Why Do UQ?

- UQ community focuses on algorithms, theory
- Applications community perspective
  - UQ is a means to an end
  - Focus on decision making
  - Value results over algorithms
  - Value ease of interpretation over theory
- Challenge problems for two communities share *similar ideas*, but are focused differently



Risk Informed Decision Making

- Progression of required info:
  - Predictions → Need Modeling and Simulation
  - Variability/Uncertainty → Need UQ
  - Credibility → Need Verification & Validation (V&V)

- Need an 'end-to-end' approach
  - Simulations to decision
- UQ is an important piece
  - Parametric, Model form, numerical
  - Aleatoric, epistemic uncertainty

Motivation & Vision

- V&V field is developing fast
  - PSAAP schools beginning to use V&V
  - ASME V&V Symposium, engineering journals
  - Workshops help move the field forward
- **Vision** – series of workshops
  - Range of topics: Verification, Validation, UQ
  - Range of audiences: Industry, Academia, Labs
  - Range of venues/partners: ASME, USACM, SIAM

  → Increase awareness, interest, and innovation

Outline

- *Motivation and Vision*
- What is Verification & Validation
- Workshop
  - Timeline
  - Initial Plans
- Draft of a Challenge Problem
  - Concepts & Expectations
- What's Next?

V&V on One Slide

- Goal: gather evidence that predictions & UQ are credible
- Start w/ math model of some phenomenon
- Is the code implementing the math model? **Code Verification**
- Is the solution being calculated accurately? **Solution Verification**
- What are the unknowns?

  What impact do they have on predictions? **UQ**
- Do the predictions match reality? **Validation**
- What is the acceptable use of the predictions? **Decisions**

What is the State of the Art?

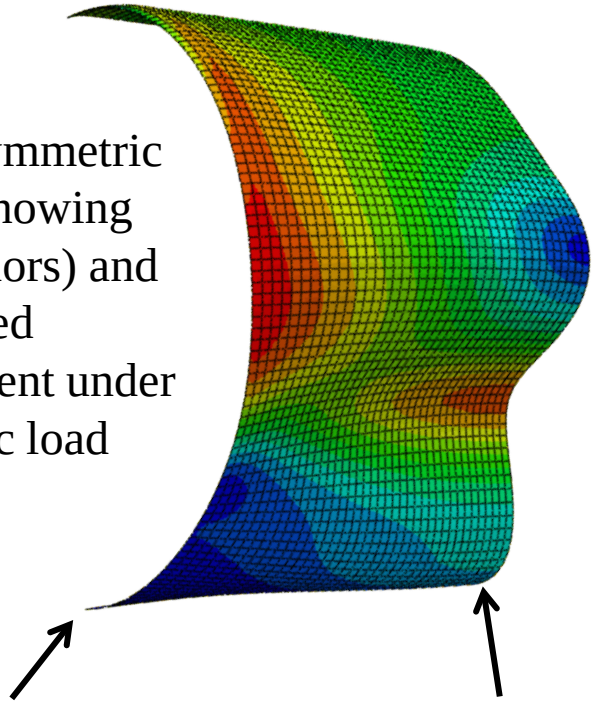
Gaps: synthesis of methods, interpretation of results

- "Aggregation" of uncertainty
  - Combine uncertainty of QoI due to multiple sources
  - Parametric uncertainty
  - Experiment-related uncertainty
  - Model form uncertainty
  - Numerical uncertainty
- Decision making with V&V/UQ information
- "Relevancy" of information throughout a hierarchy of analyses – Future topic

Green color = V&V/UQ feature of interest

The Problem

- Storage tank
- Pressure and liquid load
- One tank fails from tensile overload



Quarter symmetric cylinder showing Stress (colors) and exaggerated displacement under hydrostatic load

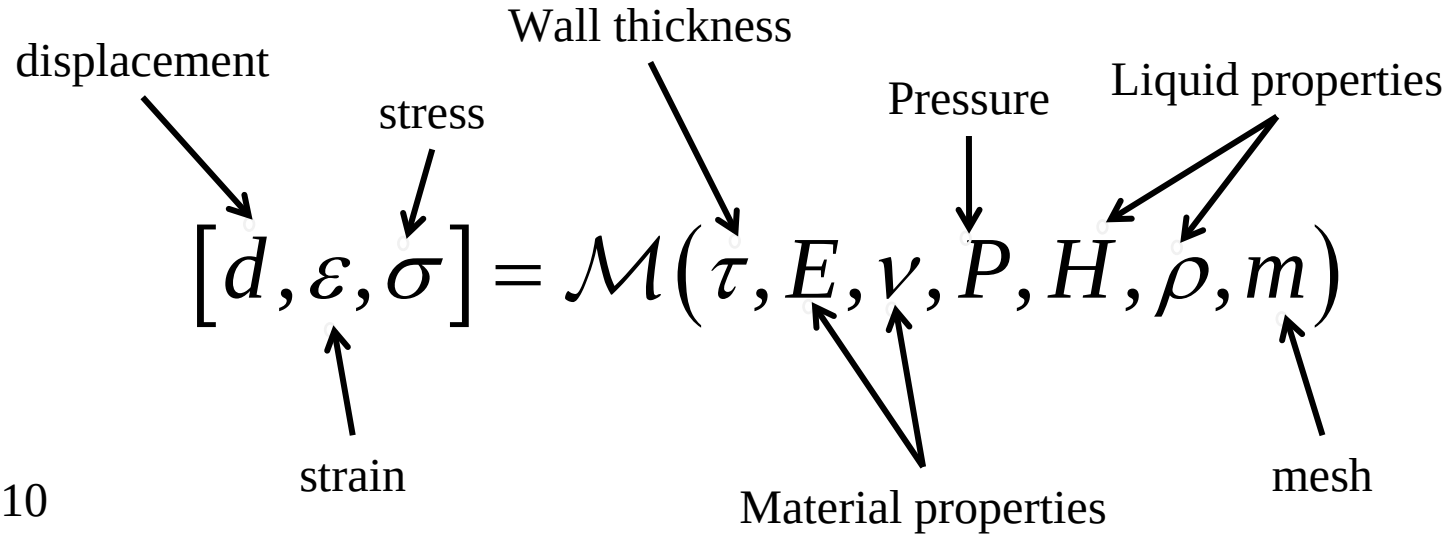
- Use test data and modeling to determine the probability of failure
- Decide whether to retire all tanks

Problem Features

- Relevant: Multiple levels → V&V hierarchy
- V&V/UQ topics: require calibration, solution verification, uncertainty quantification, validation, aggregation
- 'End-to-end' problem
  - Data and models → prediction, uncertainty, credibility → Decision informed by Modeling and Simulation
  - "Realistic", intuitive, and interesting story
- Physics based, but no physics expertise required
  - Computationally affordable; unclassified, unlimited release

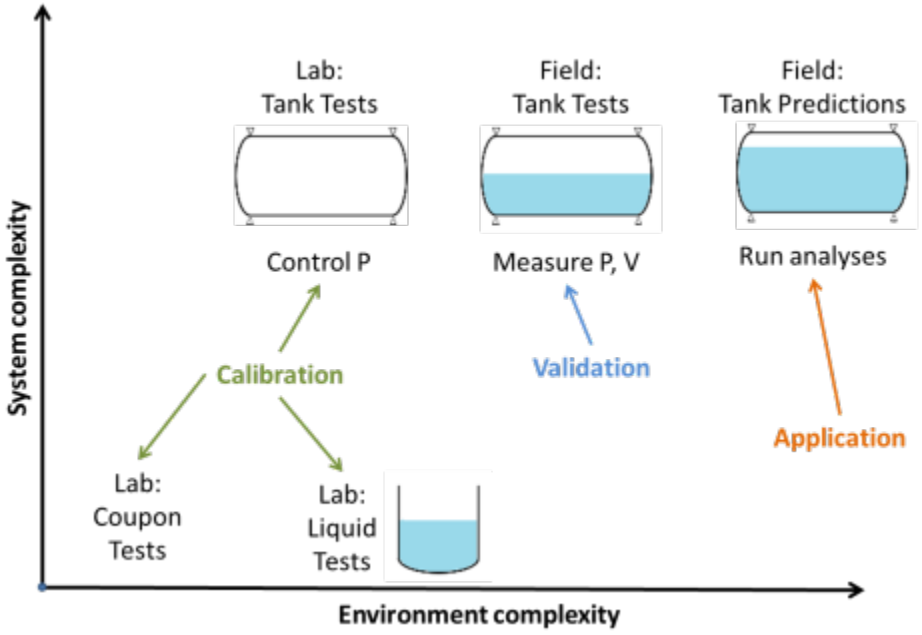
System Model Features

- Runs quickly → Not limited by methods
- Physically intuitive
  - Pressure + Liquid load → Displacement, strain, & stress
- Non-ideal convergence behavior (**solution verification**)
- Parameters and mesh interaction → Non-trivial **UQ**
- Modeling limitations
  - Calibration of parameters w/ known **model form error**



The Story → V&V Hierarchy

- Intended Use: Predict Probability of Failure under a range of scenarios
- Establish credibility of models → V&V Hierarchy



Domains: Calibration Validation Application

- Physics level
  - Measurement limitations, Variation in materials → **Parametric uncertainty**
- System level (Full tank)
  - Combine all sources of uncertainty → **Aggregation**
  - Deal with **aleatoric & epistemic uncertainty**

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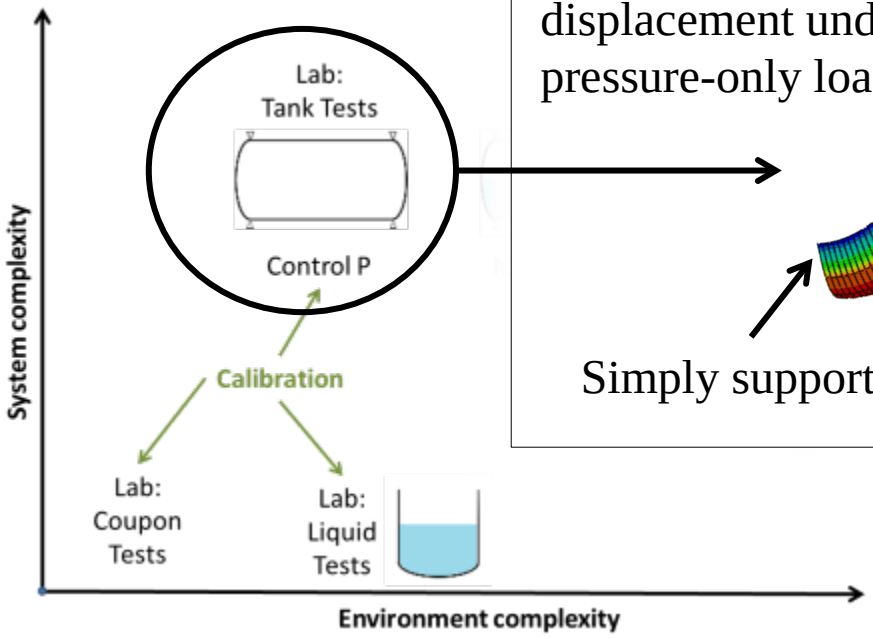
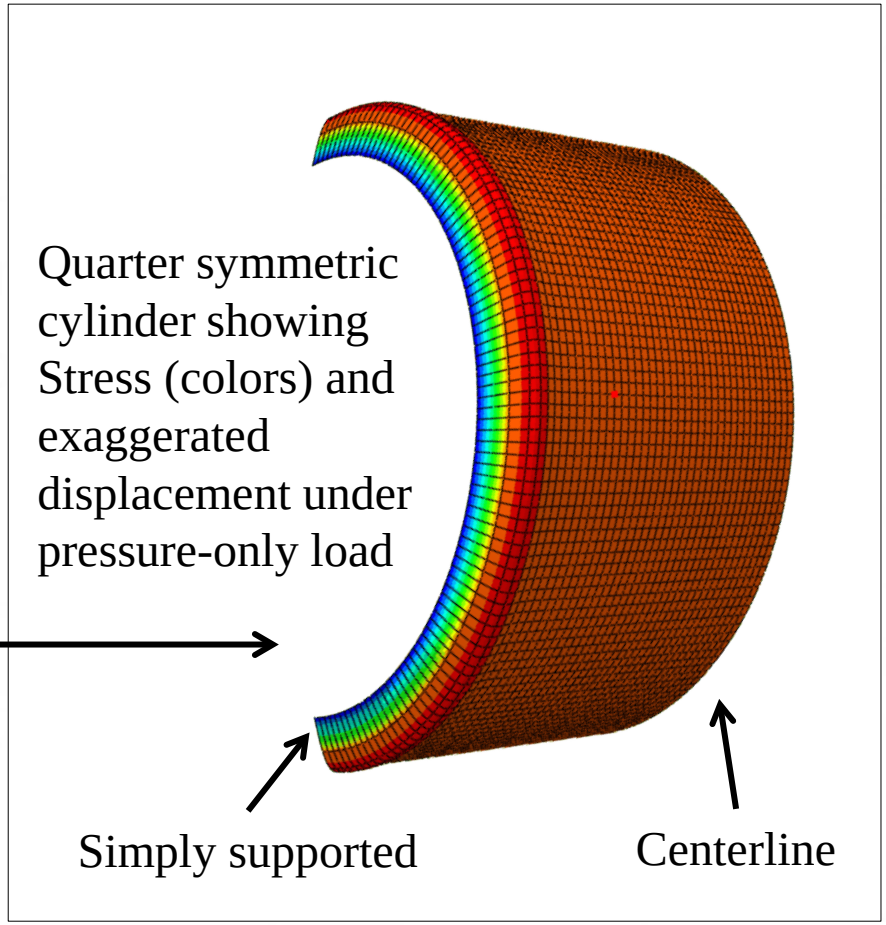
- Intended Use: F
  range of tempe
- Establish credi





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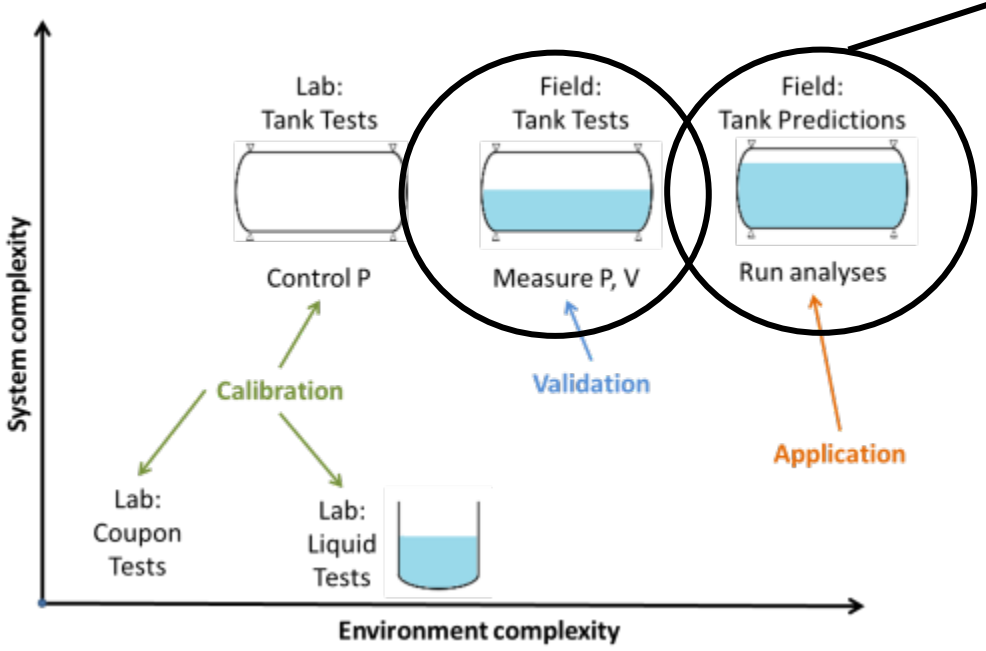
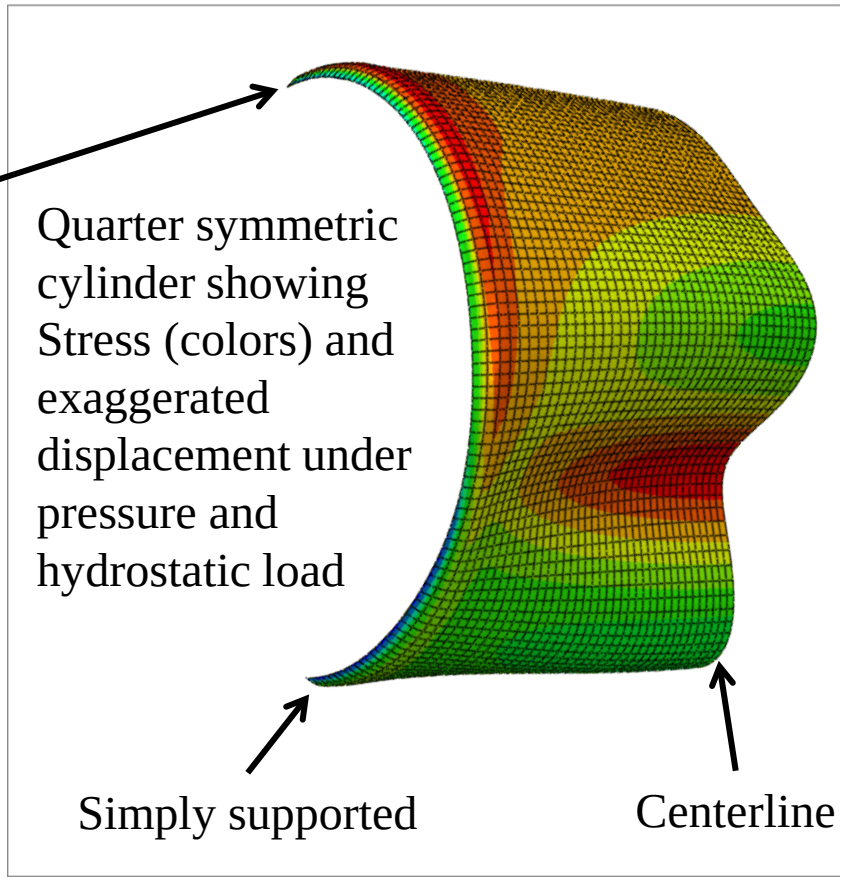
Domains: Calibration Validation Application

The Story → V&V Hierarchy

- Intended Use: Predict Probability of Failure at a range of temperatures
- Establish credibility of models →



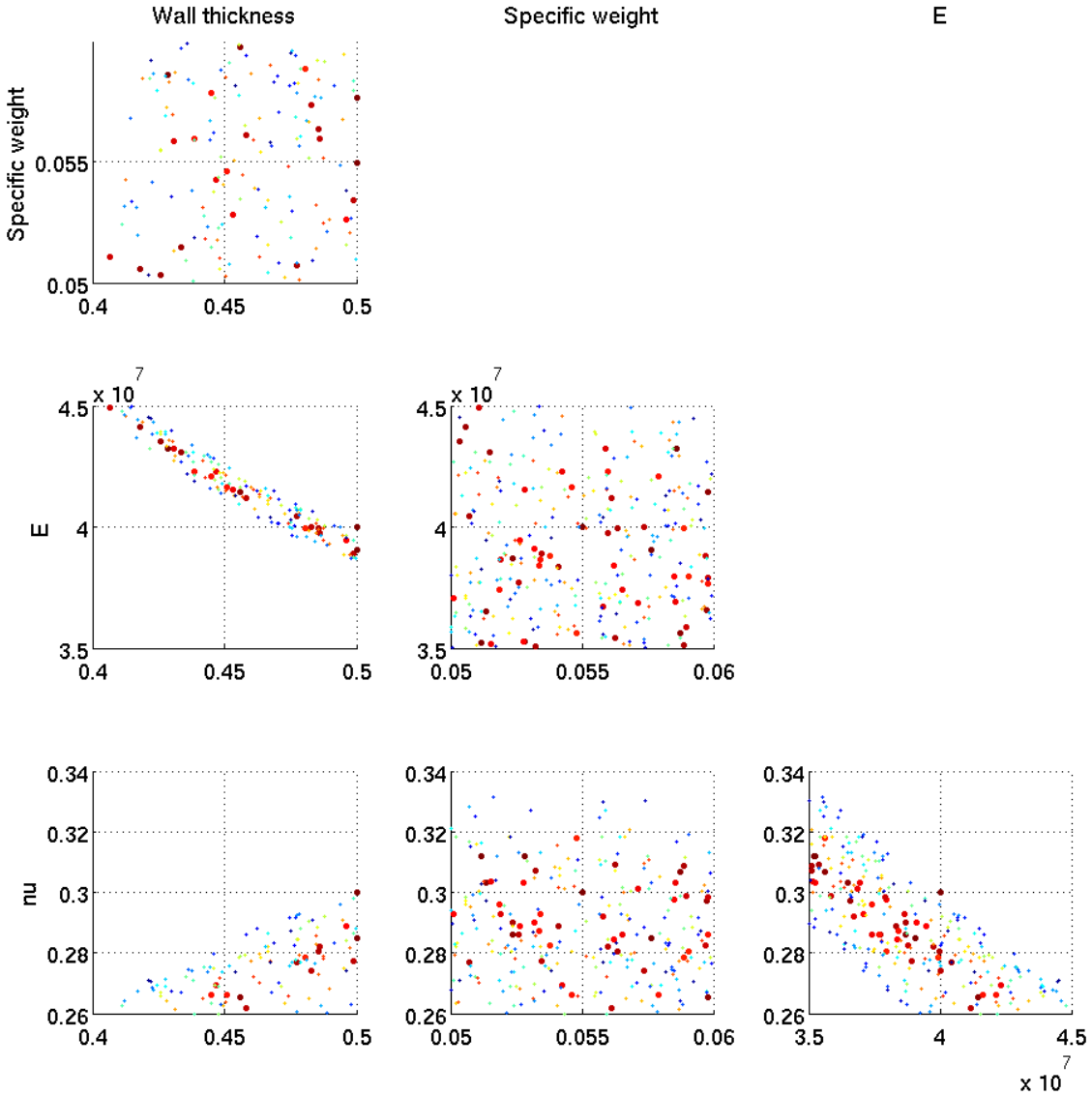


Domains: Calibration Validation Application

Problem Highlights

- Calibration
  - Legacy data on material parameters
  - Lab tests and controlled tank experiments
  - Physics model with multiple meshes
  - Deal with parametric & numerical uncertainty and model form error
- Validation
  - Limited, noisy data from uncontrolled experiments
  - Compare simulations and experiments
  - Handle aleatoric and epistemic uncertainty
- Experimental data generated from a “truth” model

Calibration – Mesh1



- Parameter Sampling
- Noiseless data
- Compute likelihoods

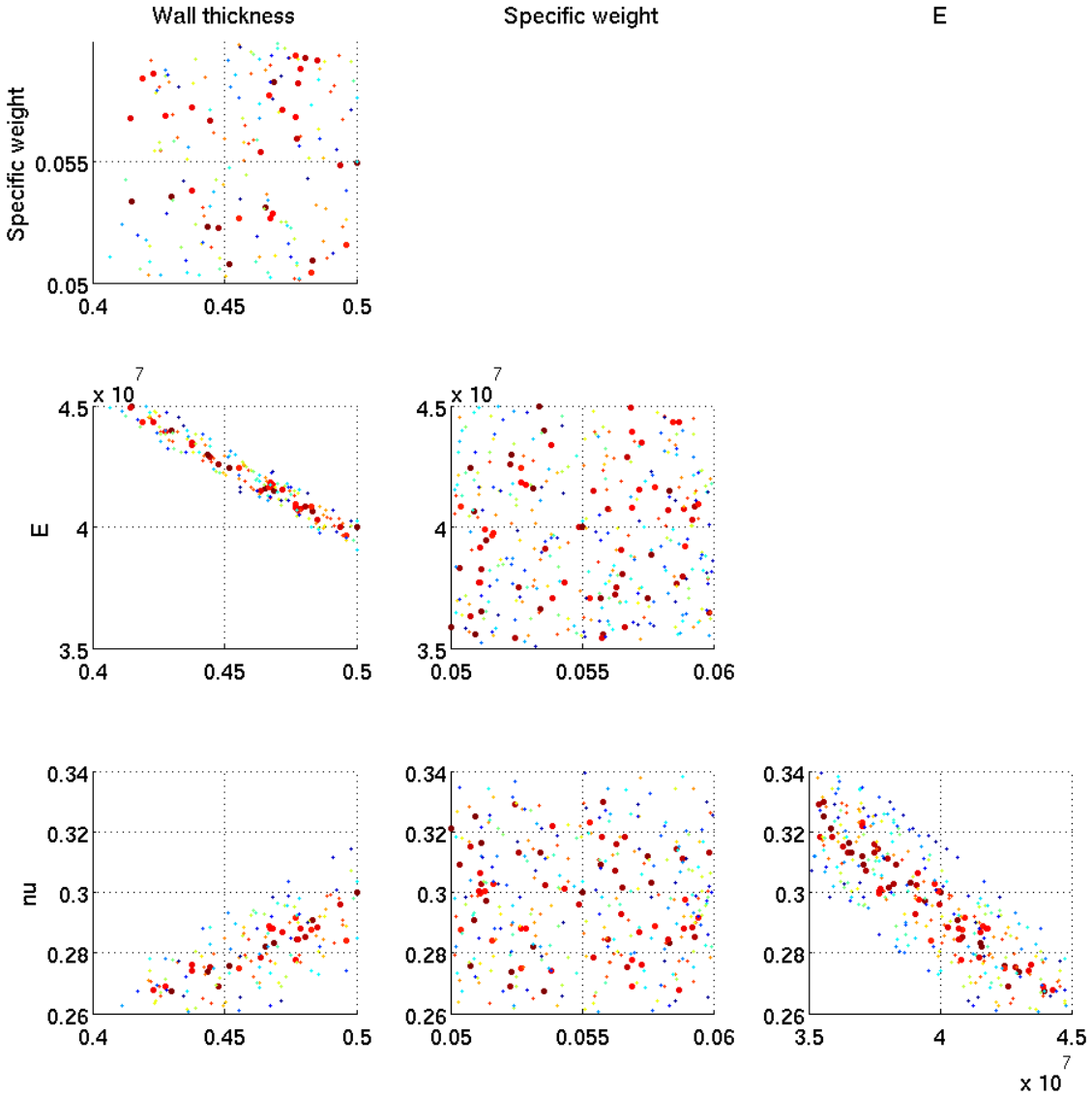
$$\sum_i \left(\mathcal{M}(\tau, E, \nu, P_i, \rho, m) - Data_i\right)^2$$

  - Red = high
  - Blue = lower

→ Mesh dependence

- Also – rate of convergence depends on parameter values
- How to calibrate?

Calibration – Mesh2



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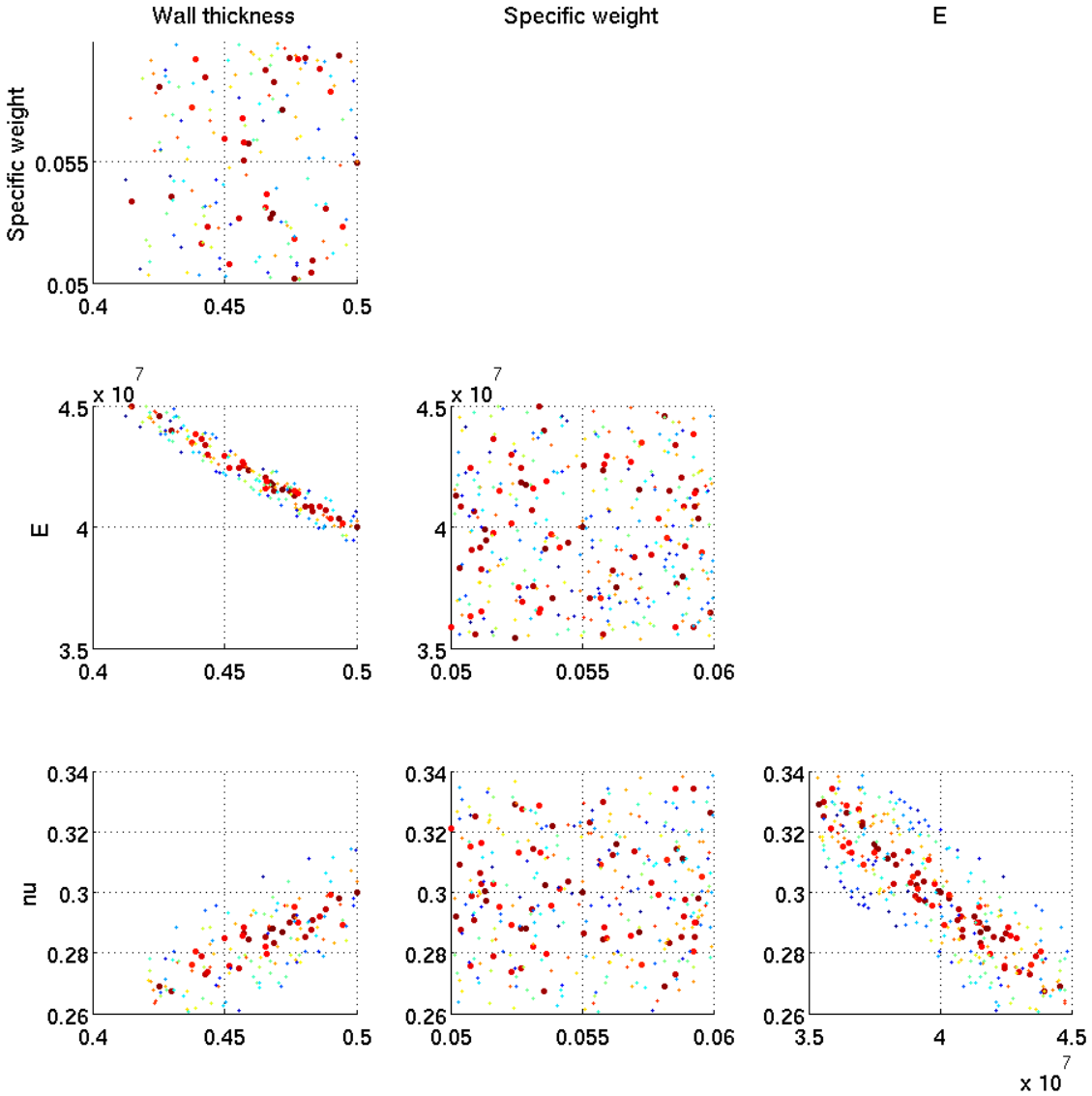
Calibration – Mesh3



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→ Mesh dependence

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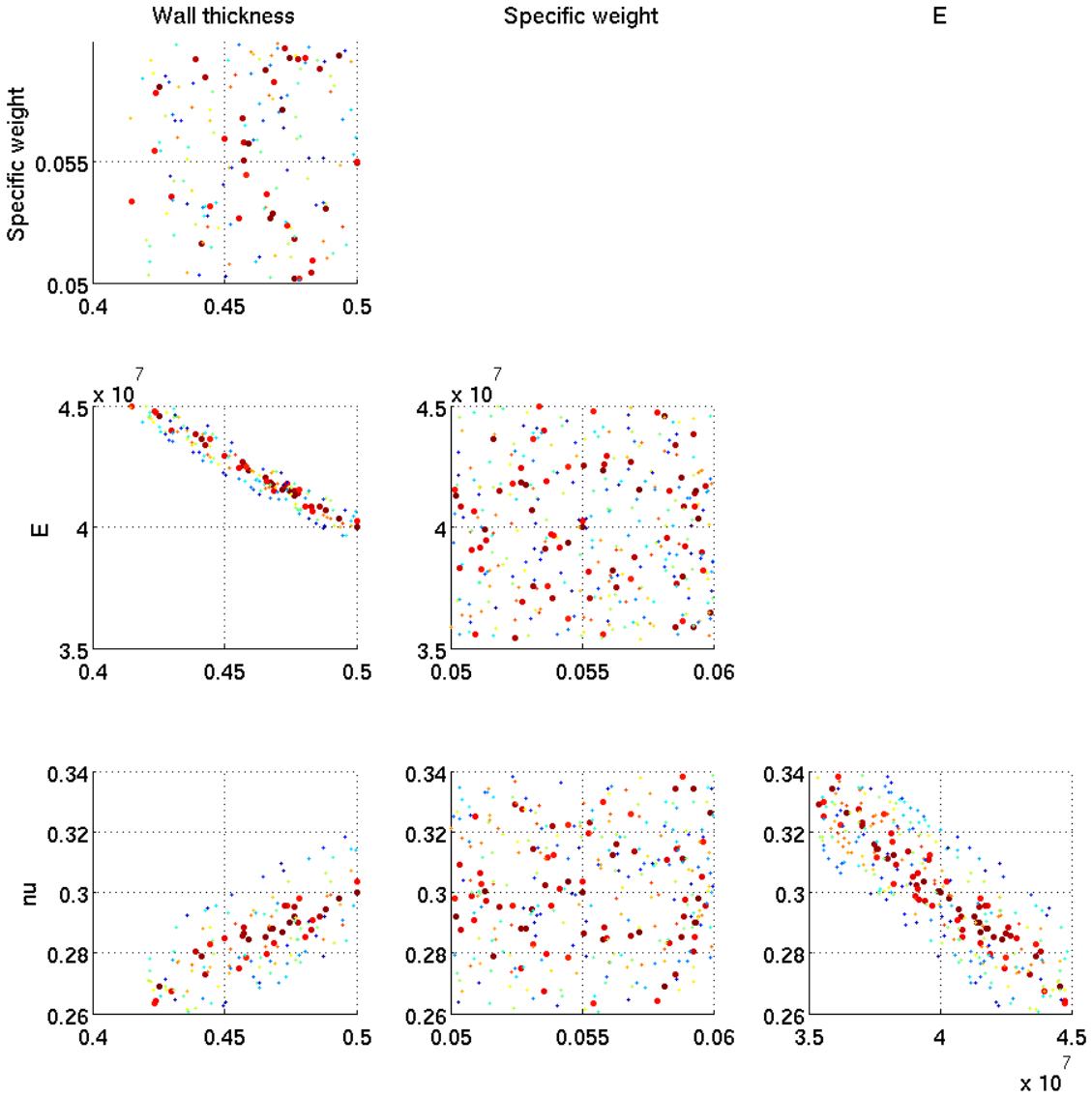
Calibration – Mesh4



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- Noiseless data
- Compute likelihoods

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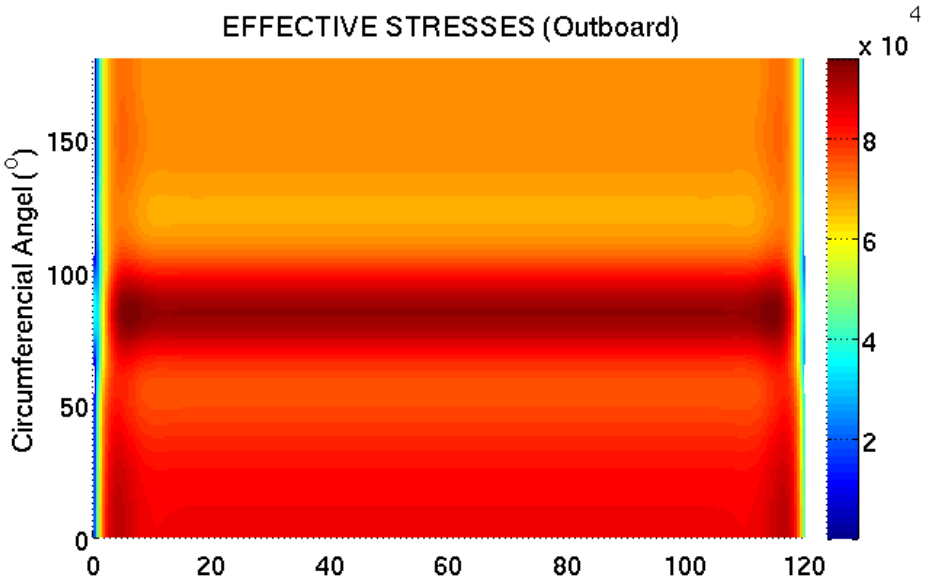
→ Mesh dependence

- Also – rate of convergence depends on parameter values
- How to calibrate?

Prediction

- Compute P (failure)
  - Based on stress
  - No data for this quantity
- Utilize
  - Available failure data
  - Aggregated uncertainty
  - Validation conclusion
- Make a decision



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Expectations

- Individual steps are straightforward
- Not limited by # of model evaluations
- Many choices: how to treat uncertainty, how to use data, how to assess credibility, etc
- No requirements on approaches
  - Supply references, suggestions, forum for discussion
- Targeting 40 hour commitment
  - NO development of physics models
  - Open ended problem – need to limit the scope!

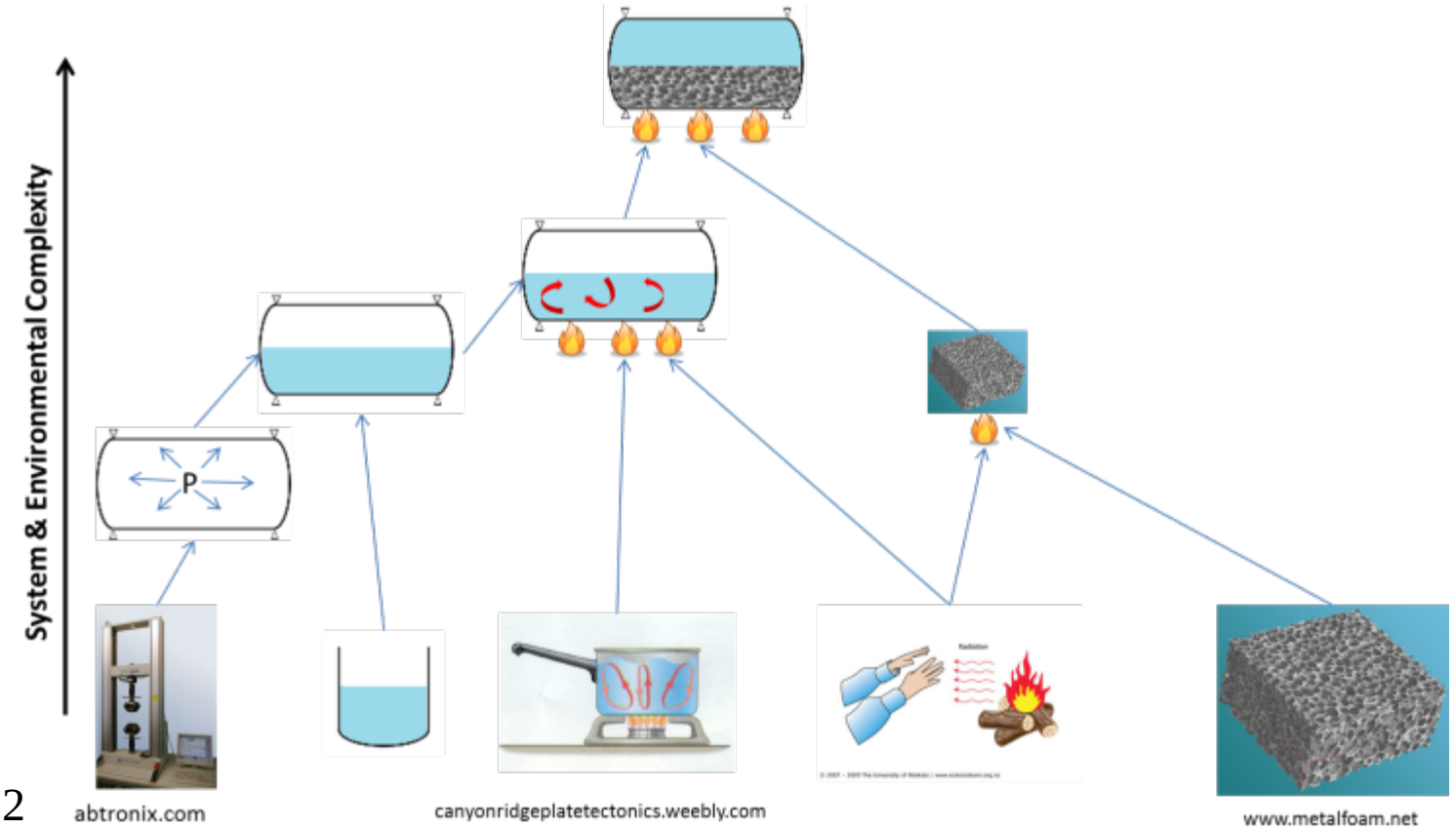
"Hidden" Features

Not explicitly asked for, to reduce problem scope

- Experiment-related uncertainty
  - Unknown experiment conditions/ Imprecise measurements
  - Propagate this to the QoI → aleatoric/epistemic issues
- **Relevancy**
  - Experimental data and simulation results from Calibration, Validation, & Application domains
    - Is all the information relevant?
    - Is the model valid (for intended use)? Is it useful?
  - Can this relevancy be quantified?
  - **How does it impact credibility?**

Context: Is this an interesting problem?

- Current V&V Hierarchy → 5 steps
  - Emphasize ideas for aggregation
- Bigger picture: Pyramid view of hierarchy



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The Workshop

- Website: https://share.sandia.gov/vvcw
- Email: vvcw@sandia.gov
  - If interested in hearing more, send an email to be placed on a distribution list
- Timeline
  - Summer 2013 – Present draft problem, gather feedback
  - Fall 2013 – Finalize problem, formally announce workshop
  - Summer 2014 – Hold workshop – ASME V&V Symposium