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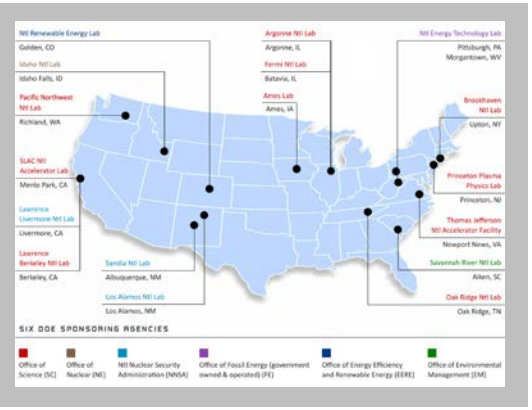

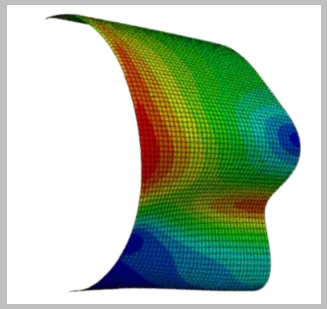

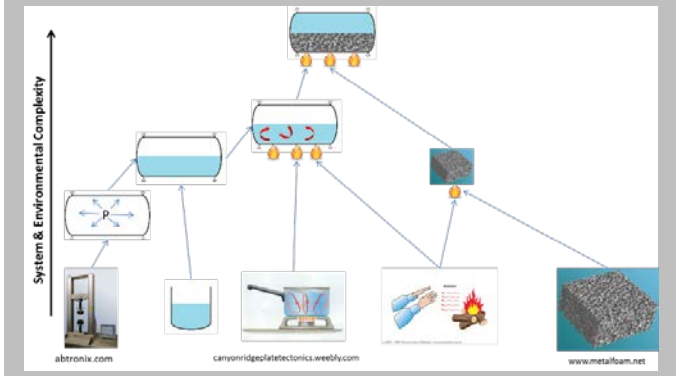

The 2014 Sandia Verification and Validation Challenge Workshop

Ken Hu

8 May, 2014

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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THE WORKSHOP

- How did we get here?
- Goals

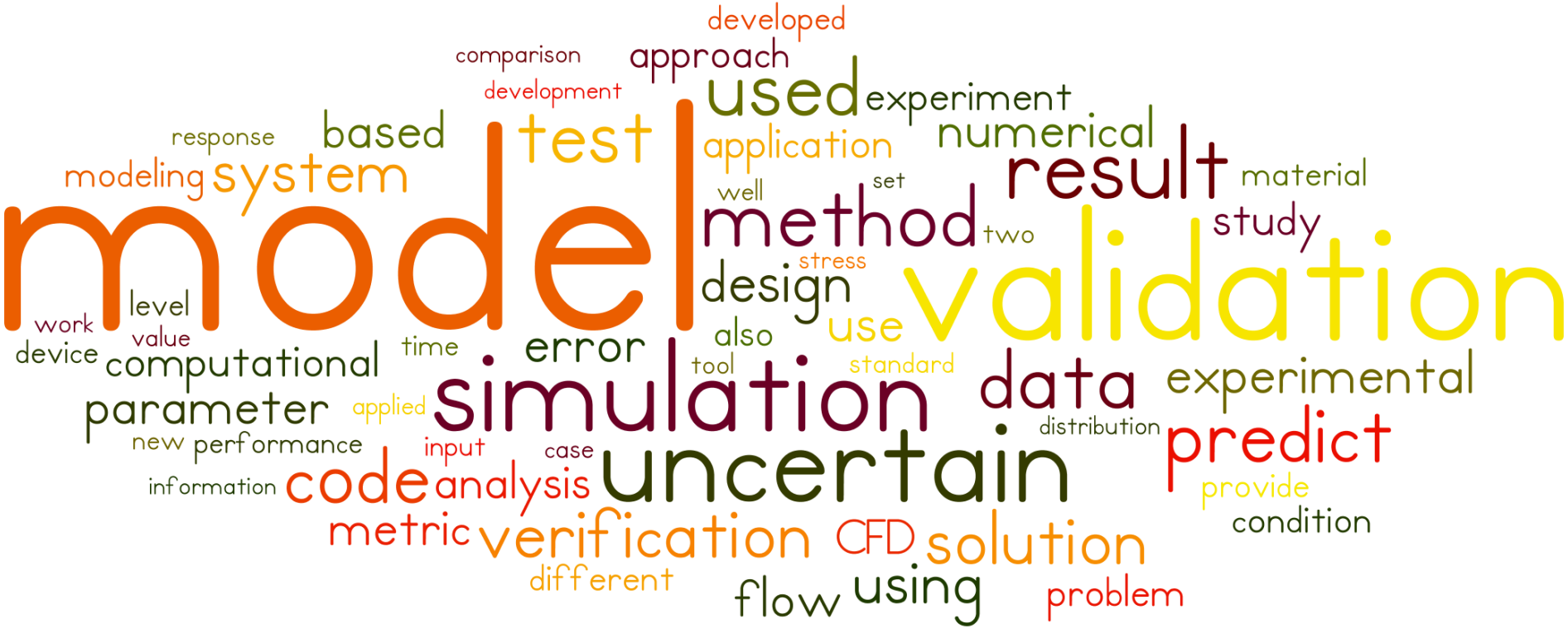
The 2014 Sandia Verification and Validation Challenge Workshop @

(Selected) History

- Foundations Series (DoD Sponsored)
- Sandia workshops
  - 2002 – Challenge problem – epistemic uncertainty
  - 2006 – Challenge 2 – connect calibration, validation, prediction
  - 2008 – methods
- AIAA/ USACM/ SIAM/ SEM/ ASME
  - V&V and uncertainty quantification talks & sessions
- ASME V&V Symposium

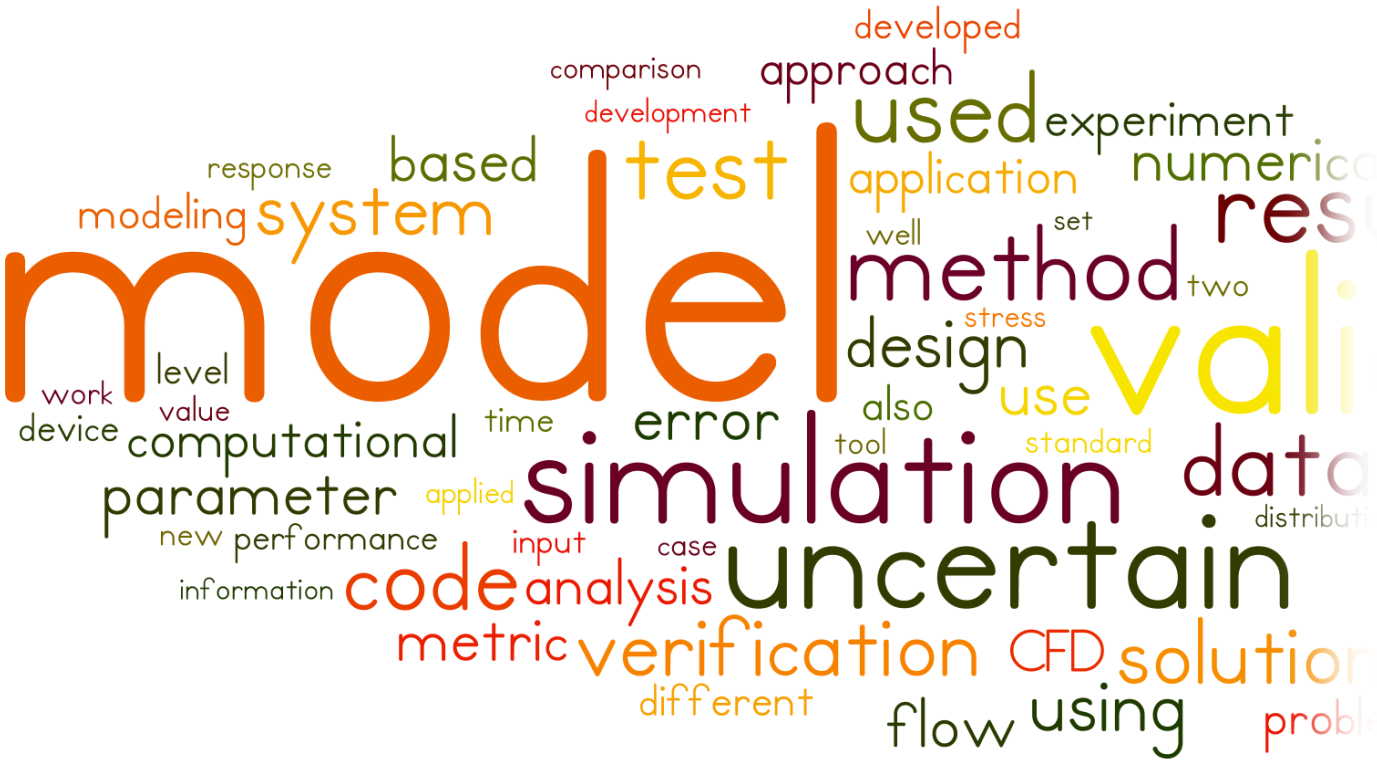
ASME V&V Symposium

- What is the community talking about?
- Three years of abstracts, summarized



ASME V&V Symposium

- What is the community talking about?



model	507
validation	298
uncertain	211
simulation	206
result	165
method	154
data	148
code	139
predict	134
verification	123
solution	121
system	113
design	105
experimental	98
decision*	116
risk*	84
credible*	62
consequence*	44

* - includes all variants

What is this all about?

- Thirty+ year history of V&V/UQ work
  - Philosophy, theory, methods, applications
- 2014 – simulations used to influence decisions

Transition V&V/UQ from R&D to production

- Much discussion of methods and demonstration
- Mentions of decision, risk, consequence

  ≠ Impact of on project outcomes

The 2014 Workshop

- Built around a challenge problem
  - Released in Fall 2013
- Participants began work 3-5 months ago
  - Seven participants presenting approaches
  - Two talks – simulations + V&V to support decision making
- Final session on Thursday – open discussions

Focus of the Challenge Problem:

How to utilize many different methods and synthesize the results?

Open questions in V&V

- How should we think about credibility/ uncertainty/ validity?
  - Can we model these concepts?
  - Can we communicate these concepts?
- How much V&V is required/ useful?
- How does V&V impact engineering projects?
- Is the community working on the right areas?

A challenge workshop is one way to focus attention

Goals for the Workshop

- Pose an "end-to-end" challenge problem
  - Data & models

    → Analysis, V&V, UQ + **???**

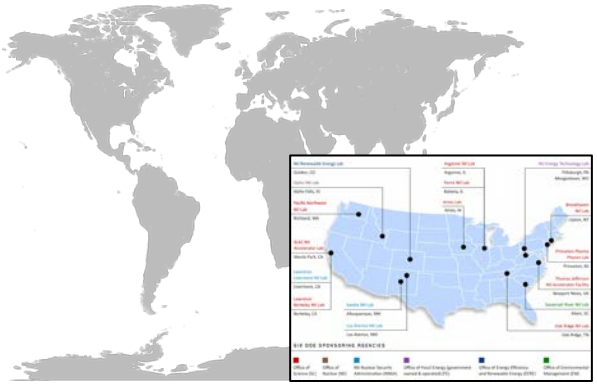
    → **decision** (or recommendation)
- Provide venue for discussions about V&V approaches PLUS "higher-level" issues
- Add to community's experience with V&V
- Restart a **workshop series**

THE CHALLENGE PROBLEM

- The story
- The challenge
- Notes about the problem

The Story of Mystery Liquid Company

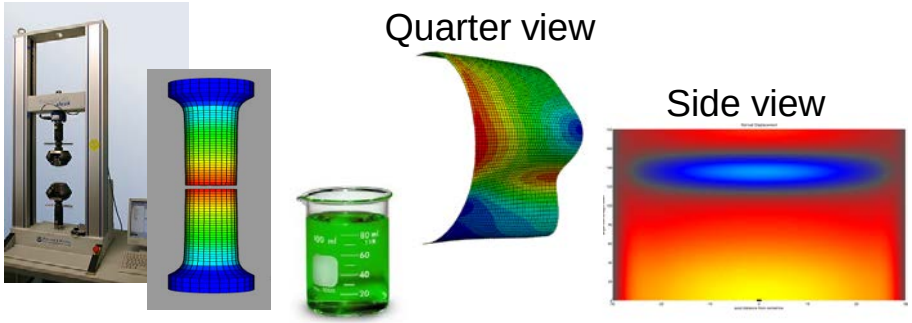
Many storage tanks, holding
Mystery Liquid under pressure



During standard safety testing,
one tank's measurements (out of many)
exceeded a safety specification

How should the company respond?
Are the tanks at risk of failure?
Must they be replaced?
No tanks have actually failed, ever.

Experimental and modeling efforts are begun



How will the evidence from experiments and simulations be integrated and used to support the final decision?

Experiments

Tank 0

Tank 0: did not pass a safety test, at removed from field and cut into pieces for measurements and materials testing

Tank dimensions

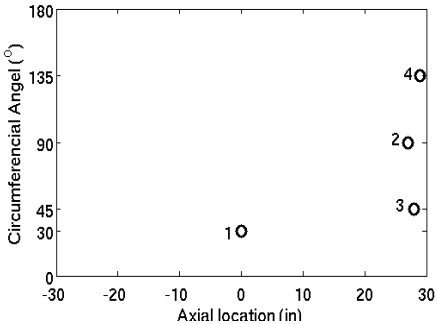
Material Properties

Tanks 1, 2

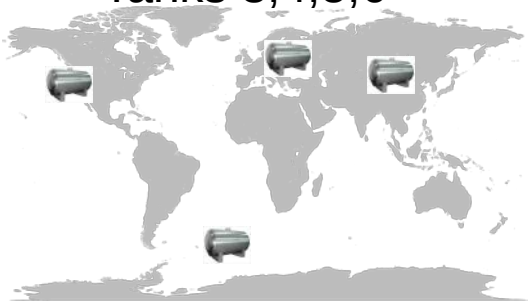
Tanks 1&2: not part of safety test, removed from field for lab testing

Tank dimensions

Wall displacement under pressure loading



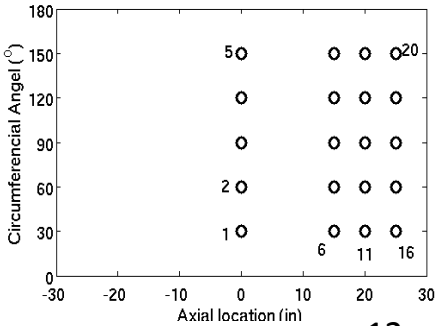
Tanks 3,4,5,6



For illustration only - not the real locations

Tanks 3-6: not part of safety test, remain in service, tested in the field

Wall displacement under pressure and liquid loading

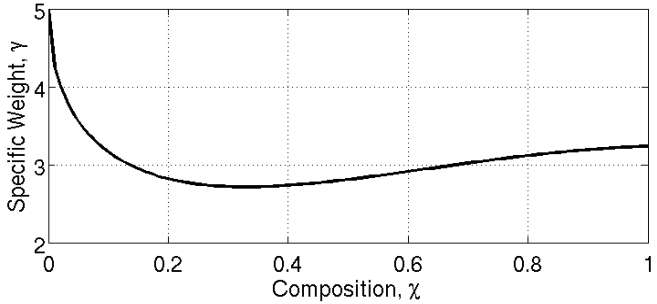


Additional Data

- Specifications from tank manufacturer
  - Tanks are decade(s) old
  - No uncertainty estimates or tolerances

- Data about the Mystery Liquid
  - Relating composition to specific weight (∝ density)

$$\gamma = \frac{7\chi}{1+0.25(\chi-0.3)^2} - 8\sqrt{\chi} + 5$$



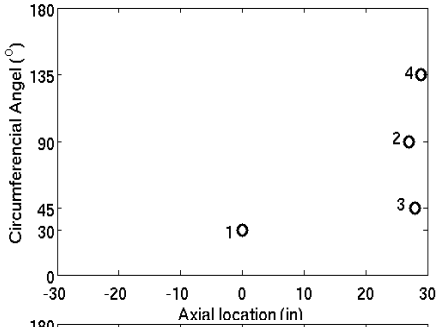
Comments on Data

- Material property data is not available
  - Only processed parameter estimates & equation of state
- Number of repeats is limited
- Many uncertainties
  - Data quality: test conditions, measurement devices, data processing, possible outliers, non-ideal choices of QoI
  - Data quantity: limited types of tests, number of tests
  - Mystery liquid equation of state is imperfect
  - Physical specimens not representative of population

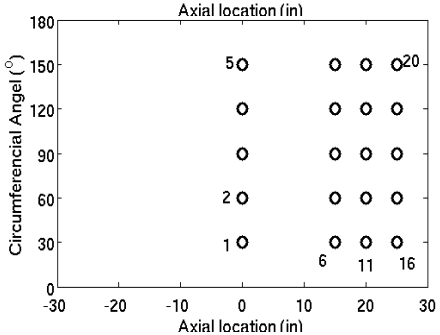
Data – summary

- Dimensions
  - Radius
  - Wall thickness
  - Length
- Material data
  - Young's modulus
  - Poisson Ratio
  - Yield stress
- Composition vs. specific weight

- Wall displacement (normal to surface)
  - Various locations
  - Various loading

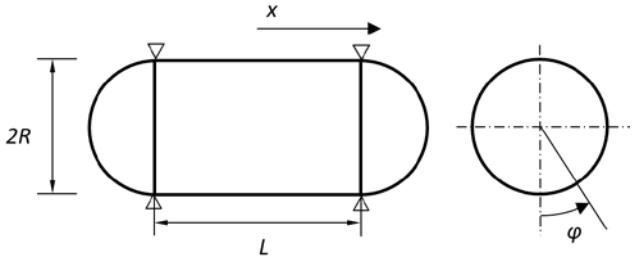


Pressure Only



Pressure and Liquid

Simulations



- Model and code implementation were supplied
  - Treated as a finite element model
  - Simplified geometry (only center section), 4 meshes created

displacement

stress

Tank Dimensions

Pressure

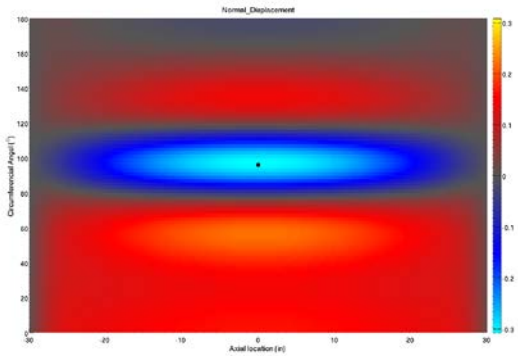
Liquid properties

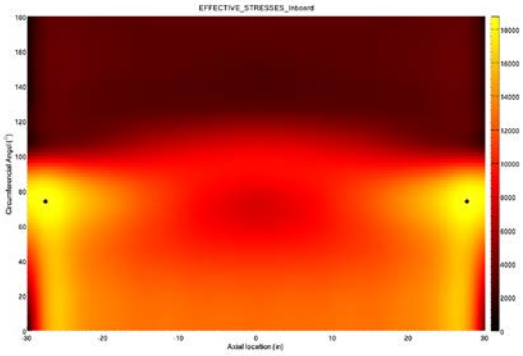
$$[d,\sigma] = \mathcal{M}(R, L, \tau, E, \nu, P, H, \gamma, m)$$

Material properties

mesh

At any axial distance x, and angle φ





Known model issues

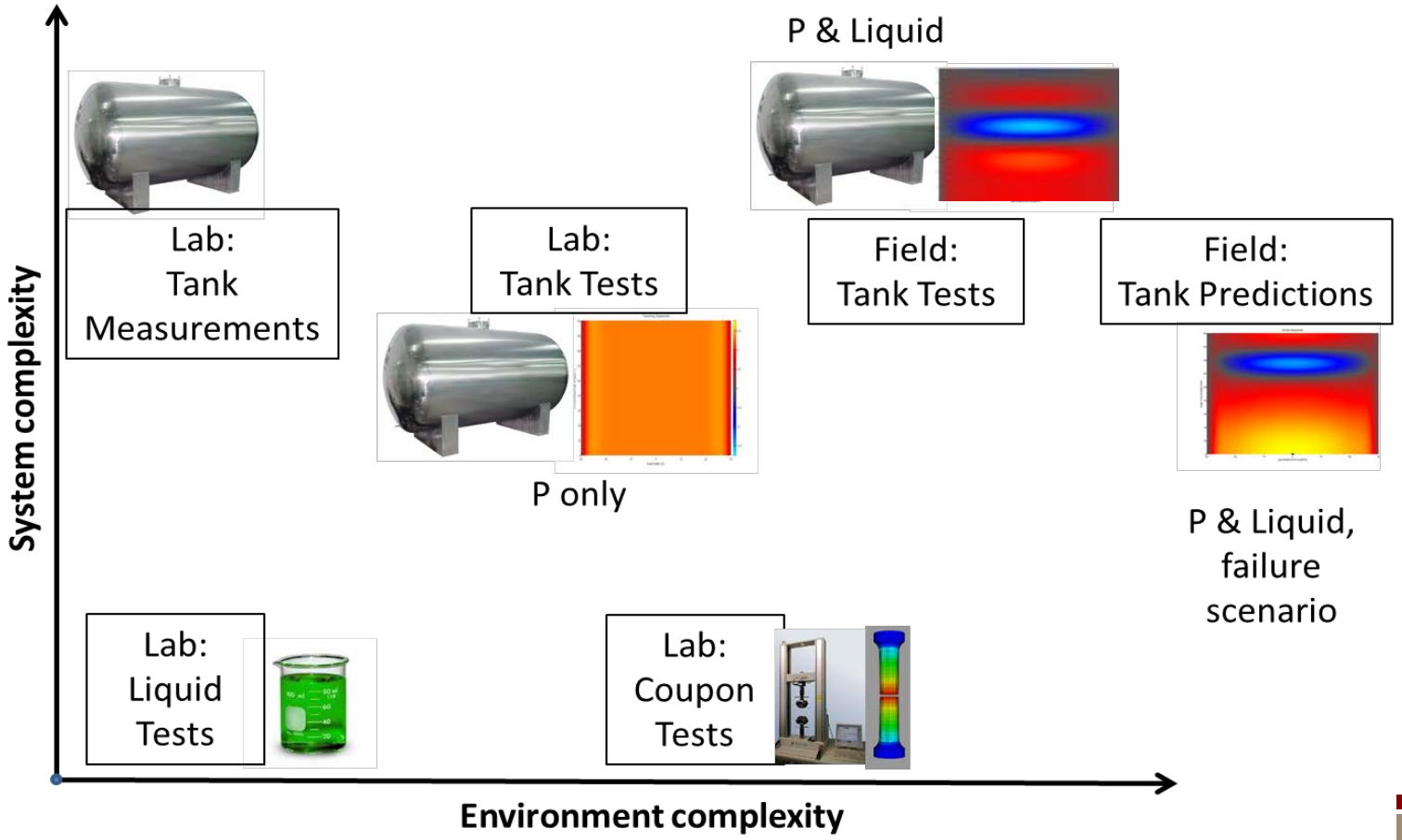
- The model only includes the center section (cylinder)
- No capability for spatial variability of inputs
- Mesh dependence
- These model limitations have unknown effects on the ability to accurately compute the responses.

The Challenge

- **Predictions + uncertainty**:
  - The ultimate product of this study will be prediction of Probability of Failure for two scenarios. In addition to a best estimate of Probability of Failure, we expect to produce uncertainty estimates.
- **Credibility Assessment**:
  - In addition to the predictions, we need to know the credibility the predicted Probability of Failure.
- **V&V Strategy**:
  - The key to providing a good credibility assessment is a logical and clearly defined strategy to gather evidence that the predictions are accurate.

Strategies/ Approaches

- How are data and simulations used?
- Need to illustrate the strategy, hierarchy of complexity

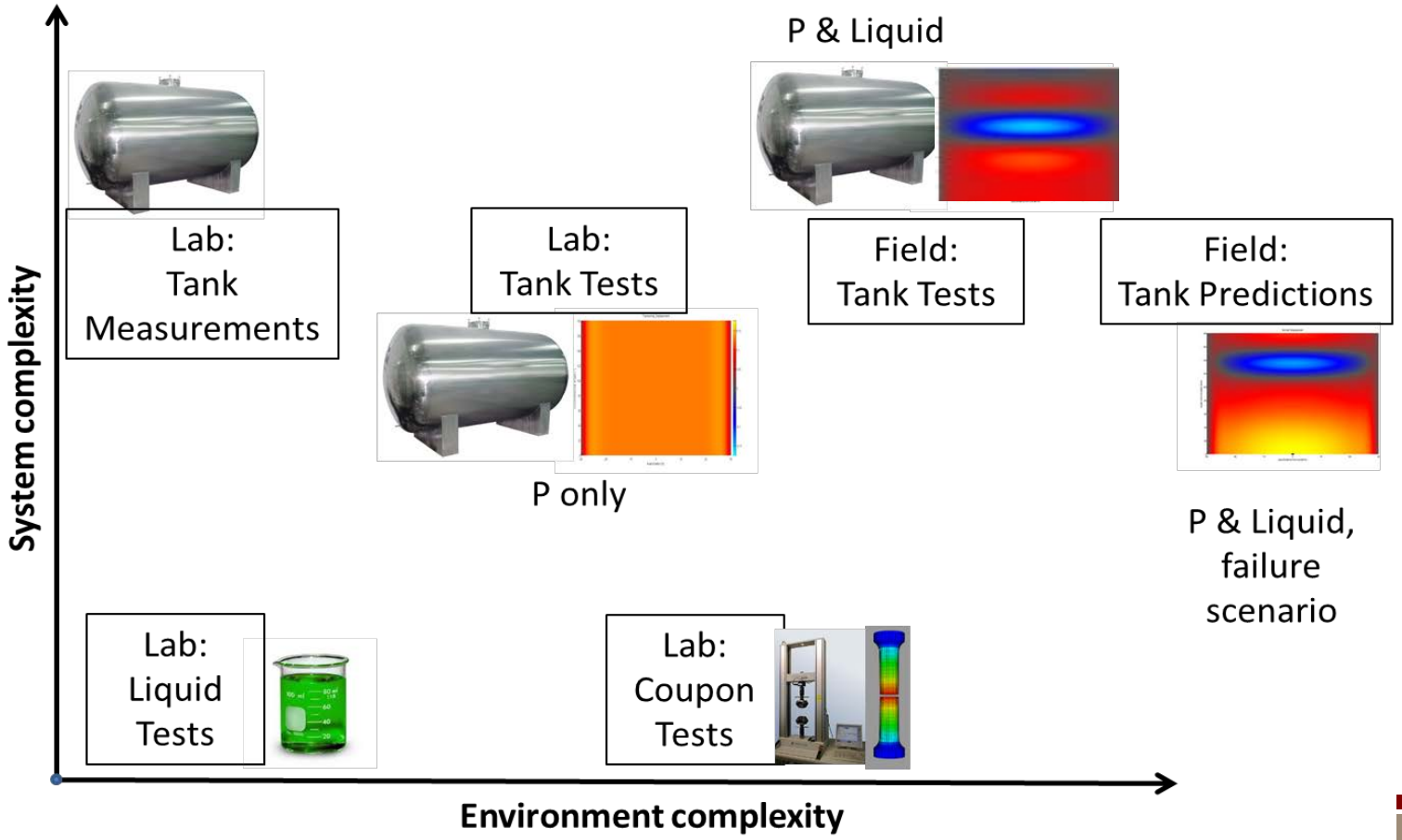


Analysis Hierarchy

- A POSSIBLE way to communicate analysis strategy
- System/ hardware levels
  - Full system (tank)
  - Material (test coupons, etc.)
- Environments
  - Uniaxial tension
  - Gas Pressure
  - Liquid load
- Match test data and simulations to nodes
- Strategy = how to use data and simulation at nodes
- Ex: calibration, validation, uncertainty characterization, solution verification, uncertainty quantification, prediction, etc.

Strategies/ Approaches

- How are data and simulations used?
- Need to illustrate the strategy, hierarchy of complexity



Prediction + Uncertainty

1. Estimate the probability of failure at the conditions of the safety test (nominal pressure, liquid height, and composition)
2. Find the boundaries of "safe operating conditions" where probability of failure $< 10^{-3}$

- Include or account for uncertainty

Credibility

- Are the simulation predictions credible?
- **After the analysis, are you ready to make a recommendation of whether to replace the tanks?**
- How do you communicate the results, uncertainty, and credibility?
- How does each V&V task contribute to the credibility of the predictions of interest?
- Does the V&V strategy as a whole add credibility?
- What is the impact of extrapolation from the validation domain?

Problem scope

- Problem statements specifies:
  - Model & code
  - Experiments & measured data
  - Quantities of Interest – wall displacement and stresses
  - Final analysis – probability of failure (based on stress)
- Code is supplied
- Participants cannot modify any of the above

- Scope is huge – assimilate data, develop a strategy, apply methods, integrate all the information…

Problem Features

- Relevant: Multiple levels → V&V hierarchy
- 'End-to-end' problem
  - Data+models → prediction, uncertainty, credibility
    → Decision informed by Modeling and Simulation
- V&V/UQ topics: calibration, solution verification, experimental and modeling uncertainty, uncertainty quantification, validation, aggregation, extrapolation to "application" domain

THEMES FOR DISCUSSION

- Gather topics during talks
- Next steps
- Future workshops

Questions for participants

- Estimate the time commitment from your group
- Estimate the number of runs and the computational cost
- Discuss how you dealt with the scope of the problem
- **If the decision maker asked for your professional opinion: are the tanks safe? What is your answer and why?**
- How would you improve your analysis?
- Would you suggest any changes to this problem or future problems?

Starter Topics

- Scope of V&V is huge
  - Too much for a single person
  - What is the most important? How to decide?
- Credibility – what does it mean?
- Culture
  - Whose job is V&V?
  - How IS V&V used? How SHOULD V&V be used?
- Next steps?
  - Publishing results, workshops, challenge problems

Acknowledgements

- Sandians – Brian Carnes, Vicente Romero, George Orient, Adam Hetzler, the Dakota team, and others
- ASME organizers, especially the V&V 20 committee
- Participants
- Many colleagues for their suggestions and help

More info:

- Website: https://share.sandia.gov/vvcw
  - Full problem statement
  - Summary handout
  - This presentation
- Email: vvcw@sandia.gov
- These will be active through FY15, then will migrate to an archive location