Verification and Validation of ICME Models

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Figure 2 Verification & Validation activities and outcomes. (Guide Figure)
Goals for this course:

- Establish Standards based Basic Vocabulary
  - “V&V activities promote team-wide communication”
- Present consensus best practices for V&V to the team in the form of lecture, discussion, and demonstration using a contextualized model.
- Introduce Standards and Tools
- Identify areas where ICME projects will encounter different challenges than have been addressed in current standards
- Contextualized Example to Illustrate core concepts of V&V and initiate discussion
- Provide References
- Feedback for improving
What we will not cover

- Prescriptive step-by-step approach
  - No one-size-fits-all solution exists
- In depth description of statistical theory
  - Proper application of statistical theory to actual engineering problems can be subtle and often counterintuitive
- Computational Tool Recommendations
  - Many excellent choices
  - User preference
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4 Follow up webinars are planned that go into the topics presented in greater detail:

1. ICME focused V&V introduction
2. V&V plan and process with examples
3. Methods: UQ and Calibration
4. End to End Case Study V&V summary with detailed review of the ICME checklists and TRL
Acknowledgments:

This course and the material contained within is the product of a large number of contributors that we would like to thank, including but not limited to:

- Southwest Research Institute
- ASME V&V 10 committee
- Metals Affordability Initiative GE-12 Team
- Dan Backman and Brad Cowles
- AFRL/RX ICME IPT and Rollie Dutton
Vision

Drive aerospace systems design by coupling computation and experiment to predict and deliver optimized materials and manufacturing solutions.

Key elements of ICME:

- Quantitative & predictive
- Computation and Experiment
- Addresses complete materials life cycle
- Integrated with system design framework
The challenge ICME addresses

- Materials are currently defined by static specs based on lengthy empirical testing. They are traditionally developed outside of the product design loop, limiting choices and opportunities.

What a tensile test looks like:
Case Study: Ni superalloy Yield strength model

Dual Microstructure Disks

Gabb et al., NASA Tech Report

Subsolvus

Supersolvus

Primary γ'

Secondary γ'

Cooling Rates

140 °F/min to 338 °F/min
Microstructure control through H.T. of disk superalloys

Temperature

~2000F

Supersolvus

Subsolvus

Time

~1500F, 8h

Subsolvus +fast cooling
primary γ' + finer structure

Supersolvus + slow cooling
coarse structure
ICME Goal:
ICMSE must deliver solutions we can trust and use.

How much confidence do we need to build in these models to use them:

• Researcher: “Will other people believe the results?”
• Engineer: “Do I believe the results enough to modify the process?”
• Engineering Project Manager: “Am I willing to bet my project (my career, my company) on these results?”
• Decision maker on high-consequence systems: “Am I willing to bet the lives of the flight crew/public safety/national security on these results?”
Validation requirements, and investment, increase with TRL...

Adapted from Cowles, B.A. and Backman, D. 2010. “Advancement and Implementation of Integrated Computational Materials Engineering (ICME) for Aerospace Applications”
“Essentially, all models are wrong, but some are useful.”

Modelers and Physicists tend to focus on whether a model is right or wrong

Engineers often ask a more useful question: How accurate is the model?

The Universe of Aristotle

Ptolemaic Model
Rome 100 AD

Modern Planetariums
Fidelity:

Current models contain an unprecedented level of detail

But How Credible Are These Models for Decision Making?
Two broad categories of uncertainty:

- **Epistemic**: lack of knowledge (property of the observer)
- **Aleatory**: inherent randomness (property of the system)

Sources of Simulation Uncertainty:
- Input Uncertainty
- Model Form Uncertainty
- Numerical Error
  - iterative error
  - discretization error

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Error: Difference between simulations results and true value

Uncertainty: When a true value is not known or defined it is a measure of possible states or values

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### Deterministic vs. Stochastic

**System:***
- Geometry
- Initial Conditions
- Physical Parameters
- Boundary Conditions
- System Excitation

\[ f(\bar{x}) \]
Transformation by the model and possibly sub models

**Surroundings:***
- Boundary Conditions
- System Excitation

**System Response Quantities:**
\[ \bar{y} \]

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**Structural Model with Deterministic Parameters**

\[ W = 100 \text{ lbs}, \ L = 10 \text{ in}, \ E = 30E6 \text{ psi}, b = 1 \text{ in}, a = 2 \text{ in} \]

**Deterministic Ranking**

- Effect on Tip Displacement
- Nominal: \( W, L, E, b, a \)

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**Structural Model with Uncertain Parameters**

- \( W \) (4% COV)
- \( L \) (0.5% COV)
- \( E \) (2% COV)

**Probabilistic Ranking**

- Effect on Tip Displacement
- \( W, L, E, b, a \)

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**Note:** COV stands for Coefficient of Variation, which is a measure of relative variability.
How is Credibility built in Modeling and Simulation?

- **Verification**
  - Credibility from understanding the mathematics
  - Are the equations being solved correctly?
  - Compare computed results to known solutions

- **Validation**
  - Credibility from understanding the physics
  - Are the correct equations being solved?
  - Compare computed results to experimental data

- **Uncertainty Analysis**
  - Credibility from understanding the uncertainties
  - How accurate is the model prediction?
  - Quantify uncertainty & variability from all sources
Verification: Process of determining that a model implementation accurately represents the developer’s conceptual description of the model and the solution to the model

Math issue: “Solving the equations right”

Validation: Process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model

Physics issue: “Solving the right equations”

Verification must precede validation; and when used, calibration must precede validation and use different data.

Heavily influenced “Guide for Verification and Validation in Computational Solid Mechanics”, ASME V&V 10-2006. This is often recommended as an excellent starting point for further investigations into the practice of V&V.
ASME V&V History and Structure

- In 1999 an ad hoc verification & validation specialty committee was formed under the auspices of the United States Association for Computational Mechanics (USACM).

- In 2001 the American Society of Mechanical Engineers (ASME) approved the committee’s charter:
  - To develop standards for assessing the correctness and credibility of modeling and simulation in computational solid mechanics.

- Committee was assigned the title and designation of the ASME Committee for Verification & Validation in Computational Solid Mechanics (PTC 60).

- With the addition of other V&V committees, an overarching committee (V&V Standards Committee) was formed and PTC 60 was changed to V&V 10.

Current Structure:

- **V&V Standards Committee in Computational Modeling and Simulation**
  - V&V 10 - Verification and Validation in Computational Solid Mechanics
  - V&V 20 - Verification and Validation in Computational Fluid Dynamics and Heat Transfer
  - V&V 30 - Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior
  - V&V 40 - Verification and Validation in Computational Modeling of Medical Devices
Current and Near Term Efforts for ASME V&V 10:

- V&V 10-2006 - Guide for Verification and Validation in Computational Solid Mechanics – Published 2006 (revision soon)
- Draft V&V 10.1 - An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics – Published 2012
- Draft V&V 10.2 - Role of Uncertainty Quantification in Verification and Validation of Computational Solid Mechanics Models – Rough draft
- Draft V&V 10.3 - Role of Validation Metrics in Verification and Validation of Computational Solid Mechanics Models – Outline
- Several others identified…
Figure 2 Verification & Validation activities and outcomes. (Guide Figure)
Validation Hierarchy

- **Validation hierarchy**
  - Breaks the problem into smaller parts
  - Validation process employed for every element in the hierarchy (ideally)
  - Allows the model to be challenged (and proven) step by step
  - Dramatically increases likelihood of right answer for the right reason

- Customer establishes intended use and top-level validation requirement

- Validation team constructs hierarchy, establishes sub-level metrics and validation requirements

- In general, validation requirements will be increasingly more stringent in lower levels
  - Full system sensitivity analysis can provide guidance
Case Study: Model Hierarchy

Alloy Composition
Final H.T. Temp

Creep model
Spreadsheet (DD) Model

PANDAT

Yield str. (x,y)
Stress relaxation (x,y)

Py/Secy/Tery γ' size
volume fraction
coherency strain vs Temp.
grain size (?)

Precipicalc (calib)

Process model

Solution T (x,y)
cooling rates (x,y)

Remaining Life (time to relax residual stress)

Feedback
Summary: V&V Process

- Design and develop the modeling and V&V plan
- Design and develop models
- Verify the model implementation
- Perform UQ and sensitivity studies to understand uncertainties
- Design validation/calibration experiments
- Perform experiments
- Assess accuracy (validation)
- Revise model/experiment
- Document the model, process, and accuracy assessments