Uncertainty Quantification and Validation Assessment

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Outline

- Background and motivation for V&V
- ASMEV&V Standards Committees
- Verification and Validation Topics
 - V&V Plan
 - V&V Process
 - Validation Hierarchy
 - Validation Experiments
 - Uncertainty Quantification
 - Validation Metrics
 - Predictive Accuracy
 - Documentation and Tracking
- Summary



Engineering Decision Analysis

- Use testing and physics-based predictions to evaluate:
 - Risk/Safety
 - Availability
 - Cost
- Intended uses
 - Improve Design
 - Minimize Cost
 - Optimize Inspections
 - Determine Warranties





Why V&V?

- Decision makers want to know:
 - Can we use this model to predict frontal barrier impacts?
 - What is the error between the model and tests?
 - How much confidence do we have in the model predictions?
 - Can we use this model to predict offset frontal barrier impacts?
- V&V can help answer these questions.



FHWA/NHTSA National Crash Analysis Center (NCAC), FEM of 2003 Ford Explorer, Version 1 (Posted 3 Jul 06).



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Current Models Contain An Unprecedented Level of Detail



How Credible Are These Models for Decision Making?



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Establishing a Predictive Capability

- 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





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Mathematical Evidence

Experimental Evidence

> Statistical Evidence

V&V Framework

 ASMEV&V 10-2006 "Guide for V&V in Computational Solid Mechanics"







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Model Verification & Validation

 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"



How NOT to do V&V





Another BAD Idea...

- Model is valid if prediction falls within experimental corridors
- Issues
 - Mismatch not quantified
 - Corridor limits are arbitrary (±1s?)
 - Reducing the quality of the experimental data improves the chance that the model is valid (not good!)





Is a Model the Same as a Code?

- Code ≠ Model
- A code is the computer implementation of algorithms developed to facilitate the solution of a class of problems (e.g., LS-DYNA)
- A model includes the conceptual, mathematical, and numerical representation of physical phenomena needed to represent a given scenario (e.g., stress analysis of a turbine blade using LS-DYNA)
- Codes are involved, but our focus is on models



Select V&V Topics

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V&V Plan

- Driven by customer
- Description of the top level model (what we ultimately want to predict)
- Intended use of the model
- System response quantities (SRQs)
- Validation metrics and requirements
- Validation hierarchy (physical and phenomena decomposition of the problem)
- Phenomenon identification and ranking table (PIRT)
- Cost and schedule constraints and expectations
- Programmatic assumptions and limitations (for example, availability of other experiments, testing, models, etc.)



No	Phenomenon	Importance (R-high, Y- med, G-low)	Adequacy (R-low, Y-med, G-high)
P1	Linear statics		
P2	Nonlinear statics		
РЗ	Nonlinear dynamics		
P4	Modal dynamics		
P5	Thermal transient		
P 6	Fragment impact		
P 7	Nonlinear dynamics and fragment impact		
P8	Threaded connection		
P9	Interference		
P10	Frictional interfaces		
P11	Assembly loads		
P12	Out of tolerance and tolerance stackup		
P13	HE Burn, gas dynamics, thermodynamics		



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Conceptual Model









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Mathematical Model



 Mathematical Model – Mathematical equations, boundary values, initial conditions, and modeling data needed to describe the conceptual model.

$$\begin{bmatrix} EI(x)y'' \end{bmatrix}'' = w(x) \quad 0 < x < L$$

$$y(0) = y'(0) = y''(L) = y'''(L) = 0$$



Mathematical Model



 Computational Model – Numerical implementation of the mathematical model, usually in the form of numerical discretization, solution algorithm, and convergence criteria.





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Verification

- The process of determining that a computational model accurately represents the underlying mathematical model and its solution
 - Code Verification
 - Context? Test Problems
 - What? Math and coding errors
 - Who? **Developers** & users
 - Calculation Verification
 - Context? Model being validated
 - What? Discretization error
 - Who? Users & developers





Validation

- Quantify the accuracy of a model by comparing model predictions to validation experiment measurements.
- Three key elements of Validation:
 - Validation Experiments
 - Validation Metrics
 - Uncertainty Quantification





What is a Validated Model?

- A model that meets the validation requirements established in the V&V plan
 - Decision maker may have other criteria to consider
- It is through the validation of the conceptual model that confidence is gained that the correct physics (mechanics) were included in the model development





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Validation Hierarchy



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Validation Hierarchy



- Validation hierarchy
 - Divides the problem into smaller parts
 - Validation process employed for every element in the hierarchy (ideally)
 - Allows the model to be challenged (and validated) step by step
 - Dramatically increases likelihood of getting the <u>right</u> answer for the right reason
- Customer establishes intended use and toplevel 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



Example Validation Hierarchy

Blast Containment Vessel





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Validation Experiments

- A validation experiment is a physical realization of an initial boundary value problem
- Purpose is to produce data that the model is expected to predict
 - Redundancy of the Data repeat experiments to establish experimental variation
 - Supporting Measurements redundant measurements to ensure data integrity and to serve as inputs to model (actual loads, for example)
 - Uncertainty Quantification model is also expected to predict measured variability
- Validation experiments are designed by both the experimentalists and the modelers
 - What's hard in the lab is easy in the model...and vice solution
 versa
- Must carefully assess whether or not existing data are suitable for validation (usually not)
- Answering the right question is challenging, both in the model and in the lab









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Uncertainty Quantification





Uncertainty Quantification

- Quantify all sources of significant uncertainty
 - Uncertainties exist in both the model and experiment
 - Reducible uncertainty (epistemic uncertainty)
 - Deficiencies that result from a lack of complete information
 - Irreducible uncertainty (aleatory uncertainty)
 - Inherent property of all physical systems
- Help design validation experiments (what to control, what not to control, what to measure, and what to let vary)
- Validation metrics will also operate on uncertain quantities



Types of Uncertainty





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Uncertainty Quantification Based on Physics-Based Model



Complexity of most physical models rules out Monte Carlo Simulation



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Why are Uncertainties Important?

Structural Model with Deterministic Parameters





Deterministic Ranking



Structural Model with Uncertain Parameters





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Validation Metrics





Validation Metrics

- A validation metric quantifies the discrepancy between model predictions and experimental data
- Typically some type of a difference measure in quantities of interest (statistics, probability distributions, etc.)
- Generally, multiple response quantities and associated metrics are better than one (right answer for the right reason)



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One Example: Area Metric

- Area difference between two cumulative distribution functions
- Global measure of agreement
 - Disagreement anywhere contributes to the metric
- A=0 means model predicted the same CDF as what was measured
- A is approximately equal to the absolute difference in the means



Oberkampf, W.L. and C.J. Roy, "Verification and Validation in Scientific Computing," Cambridge University Press, UK, 2010.



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Area Metric

- Is the model <u>adequate</u> when A=0 (i.e., perfect)?
 - Not necessarily...it just means the model is predicting the same uncertainty as what was measured
- Is there any way to improve the model when A=0?
 - Yes, but the area metric has taken us as far as it can go
- Perhaps useful to also measure how well the model is predicting possible experimental outcomes



System Response Quantity



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Second Example: Error Metric

- Absolute error between a model prediction and an experimental response quantity
 - Model prediction and experimental measurement are uncertain



 Y^{exp}

Thacker, B.H. and T.L. Paez, "A Simple Probabilistic Validation Metric for the Comparison of Uncertain Model and Test Results," AIAA SciTech, 16th AIAA Non-Deterministic Approaches Conference, National Harbor, Maryland, 13-17 January 2014. MECHANICAL ENGINEERING



 V^{mod}

Error Metric Interpretation



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Error Metric

CDF Provides Relationship between Error and Probability





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Model and Test CDFs at Various Times





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Comparison of Metrics in Time





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Predictive Accuracy

- Validation: the process of determining the degree to which a model is an accurate representation of the experiment.
- Prediction: Use of a model to calculate a response where corresponding experimental data are not available.
- Predictions are made during the course of performing validation.
 - Once compared to experimental data, however, it is no longer a prediction



Concept of the Validation Domain

- Illustration for two input parameters
- Validation process performed and passed at each validation point
- Engineering experience or intuition might suggest that predictions within the validation domain should be more reliable than predictions made outside the validation domain.
 - Safe assumption?





Validation Domain with Uncertainties

- Degree of agreement contours computed from validation metric
 - Could also be discrepancy
 - Contours are not input uncertainties
- What is the validation domain?
- Additional validations or improvements in existing validations will update the validation domain contours
- Perhaps a method to associate an accuracy with a prediction





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Documentation and Tracking

- Documentation is critical in a V&V program
 - No documentation = No credibility
 - What was done, and how to carry forward
- Predictive capability maturity model (PCMM) serves as one way to organize, measure and communicate the model development process
 - Evidence is the focus of PCMM, not adequacy of results
 - Speaks to M&S maturity like TRL's speak to hardware maturity
 - Other measurement systems proposed



- Geometric fidelity (GF)
- Physics fidelity (PF)
- Code verification (CV)
- Solution verification (SV)
- Validation (VAL)
- Uncertainty quantification (UQ)



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