Uncertainty Quantification and Validation Assessment

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Outline

- Background and motivation for V&V
- ASME V&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.
Current Models Contain An Unprecedented Level of Detail

Fidelity ≠ Accuracy

How Credible Are These Models for Decision Making?
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
V&V Framework

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

Fully Reversed
S_{max} = 54 MPa

Surface Crack Length, c (inches)

Cycles

Test (2-10)
2.25, C
Another BAD Idea…

- Model is valid if prediction falls within experimental corridors

- Issues
  - Mismatch not quantified
  - Corridor limits are arbitrary (±1σ?)
  - 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

- **V&V Plan**
  - What is the question, and how good of an answer is needed?

- **V&V Process**
  - Is the model correct and credible?

- **Validation Hierarchy**
  - Right answer for the right reason?

- **Validation Experiments**
  - What quantities need to be measured (or obtained)?

- **Uncertainty Quantification**
  - What are the sources and impact of uncertainty in model and test?

- **Validation Metrics**
  - How will the model predictions be compared to experimental data?

- **Predictive Accuracy**
  - What accuracy (and confidence) can be associated with a prediction using a validated model?

- **Documentation and Tracking**
  - How to track and communicate progress?
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.)
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Conceptual Model

- Conceptual Model – Collection of assumptions and descriptions of physical processes representing the solid mechanics behavior of the reality of interest from which the mathematical model and validation experiments can be constructed.
Mathematical Model

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

\[
\left[ EI(x) \frac{d^4 w}{dx^4} \right] = w(x) \quad 0 < x < L
\]

\[
y(0) = y'(0) = y''(L) = y'''(L) = 0
\]
Mathematical Model

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

Approach: Bottom-up guided by sensitivity analysis of (un-validated) full system model
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 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
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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 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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Quantification of all significant uncertainties in both model and test
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

- Aleatory
  - Inherent randomness
  - Property of the system

- Epistemic
  - Lack of knowledge
  - Property of the modeler

- Recognized
  - Model form error
  - Numerical solution error
  - Limited samples

- Blind
  - Programming errors
  - Modeling errors
  - Poor decisions

Error
- Deviation from the true value
- True value typically unknown
- Model as an epistemic uncertainty
Uncertainty Quantification Based on Physics-Based Model

Input Uncertainties
- Material Properties
- Loadings
- Boundary Conditions

Model

Response and Failure Model

Output Uncertainty
- Reliability
- Life

Complexity of most physical models rules out Monte Carlo Simulation
Why are Uncertainties Important?

Structural Model with Deterministic Parameters

\[ \delta = \frac{3WL^3}{2Eba^3} \]

\( W = 445 \text{ N}, \quad \text{L} = 25.4 \text{ cm}, \quad E = 207 \text{ GPa}, \quad \text{b} = 2.54 \text{ cm}, \quad \text{a} = 5.08 \text{ cm} \)

Deterministic Analysis

Effect on Tip Displacement

Deterministic Ranking

Structural Model with Uncertain Parameters

Probabilistic Analysis

Probabilistic Ranking

Effect on Tip Displacement

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

445 N  25.4 cm  206843 MPa

b (0.5% COV)  a (0.05% COV)

2.54 cm  5.08 cm
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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).
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

\[ A = \int_{-\infty}^{\infty} |F_{y_{\text{mod}}} (y) - F_{y_{\text{exp}}} (y)| \, dy \]

Area Metric

- Is the model **adequate** 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
Second Example: Error Metric

- Absolute error between a model prediction and an experimental response quantity
  - Model prediction and experimental measurement are uncertain
    \[ Z = \frac{Y^\text{mod} - Y^\text{exp}}{Y^\text{exp}} \quad \text{or} \quad Z = \frac{Y^\text{mod} - Y^\text{exp}}{E[Y^\text{exp}]} \]
    
    \[ p = P(|Z| \leq z) \] Probability that the error will not be exceeded
  - Validation Requirement
    \[ p < p_r \quad \text{or} \quad z < z_r \]

Error Metric Interpretation

90% probability that the error will not be greater than 15.6%

\[ P\left(\left|Z\right| \leq z\right) = p \]

\[ Z = \frac{Y_{\text{mod}} - Y_{\text{exp}}}{Y_{\text{exp}}} \]
Error Metric

CDF Provides Relationship between Error and Probability

10% probability the error will not be greater than 10%

90% probability the error will not be greater than 553%
Model and Test CDFs at Various Times

- **t=0.005 s**
- **t=0.01 s**
- **t=0.015 s**
- **t=0.02 s**
- **t=0.025 s**
- **t=0.03 s**
- **t=0.035 s**
- **t=0.04 s**
Comparison of Metrics in Time

- Area Metric
- Z-metric, p=90%
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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)
Summary

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