Concepts and Practice of Verification, Validation, and Uncertainty Quantification

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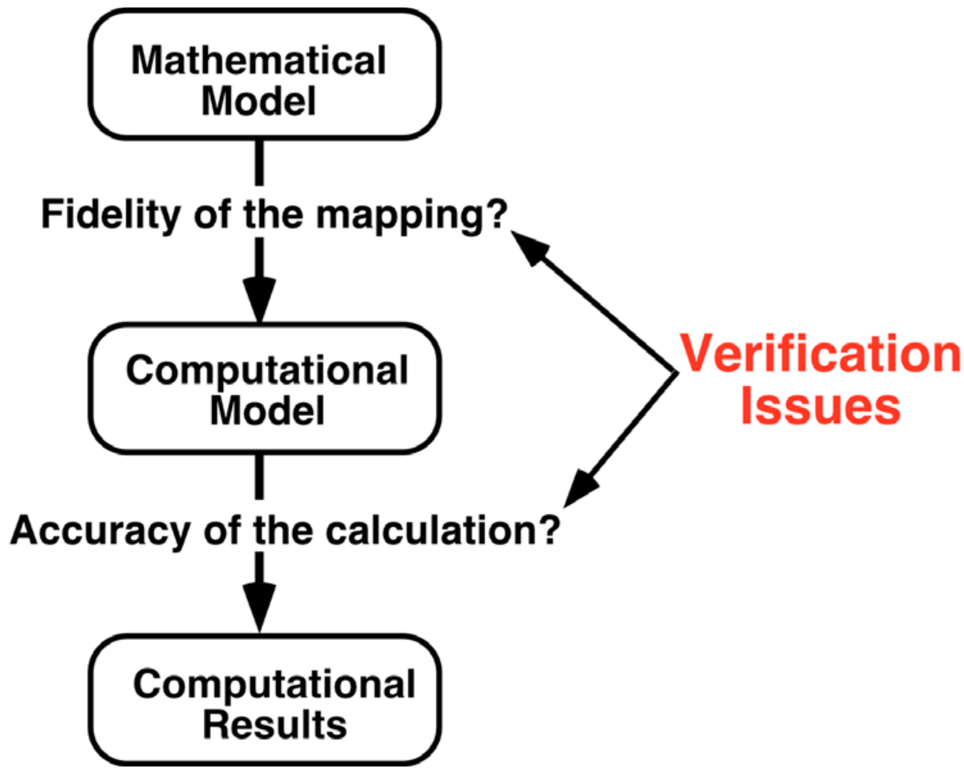
Outline

- Code verification
- Solution verification
- Model validation
- Validation metrics
- Predictive uncertainty
- Concluding remarks

Formal Definition of Verification (DoD, AIAA, ASME)

Verification: **The process of determining that a computational model accurately represents the underlying mathematical model and its solution.**

Verification deals with mathematics and software engineering



Two Types of Verification Processes

- **Code Verification: Verification activities directed toward:**
  - **Finding and removing mistakes in the source code**
  - **Finding and removing errors in numerical algorithms**
  - **Improve software using software quality assurance practices**
- **Solution Verification: Verification activities directed toward:**
  - **Assuring the correctness of input data for the problem of interest**
  - **Estimating the numerical solution error**
  - **Assuring the correctness of output data for the problem of interest**

Code Verification Activities

- **Two types of code verification activities:**
  - **Software quality assurance practices**
  - **Numerical solution testing procedures**

- ***Order of accuracy (convergence)* of the computer code**
  - **Demonstrate that the discretization error** $\varepsilon_h = u_h - u_{exact}$ **reduces at proper rate with systematic mesh refinement:**

$$p = \frac{\ln(\varepsilon_{rh}/\varepsilon_h)}{\ln(r)} \qquad r > 1$$

  - **Systematic refinement requires uniform refinement over the entire solution domain**

- **Approach requires an exact solution to the mathematical model to *evaluate* the error**

Code Verification: Derivation of Exact Solutions

Two approaches for obtaining exact solutions to the mathematical model: code-to-code comparisons are unreliable

- **Closed form analytical solutions – given a properly posed PDE and initial / boundary conditions:**
  - **Exist only for simple PDEs**
  - **Do not test the general form of the complete mathematical model**
- **Method of Manufactured Solutions (MMS)**
  - **Given a PDE** $L(u) = 0$
  - **Find the modified PDE which the solution satisfies**
    - **Choose an analytic solution,** $\hat{u}$**, e.g., sinusoidal functions**
    - **Operate** $L(\bullet)$ **onto the solution to give the source term:** $L(\hat{u}) = s$
    - **New PDE** $L(u) = s$ **is then numerically solved to get** u_h
  - **Discretization error can be *evaluated* as:** $\varepsilon_h = u_h - \hat{u}$

Solution Verification

- **In solution verification, the various sources of numerical error must be *estimated:***
  - **Round-off error**
  - **Iterative error**
  - **Discretization error**
- **Numerical error should be estimated for:**
  - **Each of the system response quantities (SRQs) of interest in the simulation**
  - **For the range of input data conditions that are simulated**
  - **Preferably, the "worst case" input data conditions are used to estimate the numerical error**

Solution Verification: Classification of Discretization Error Estimators

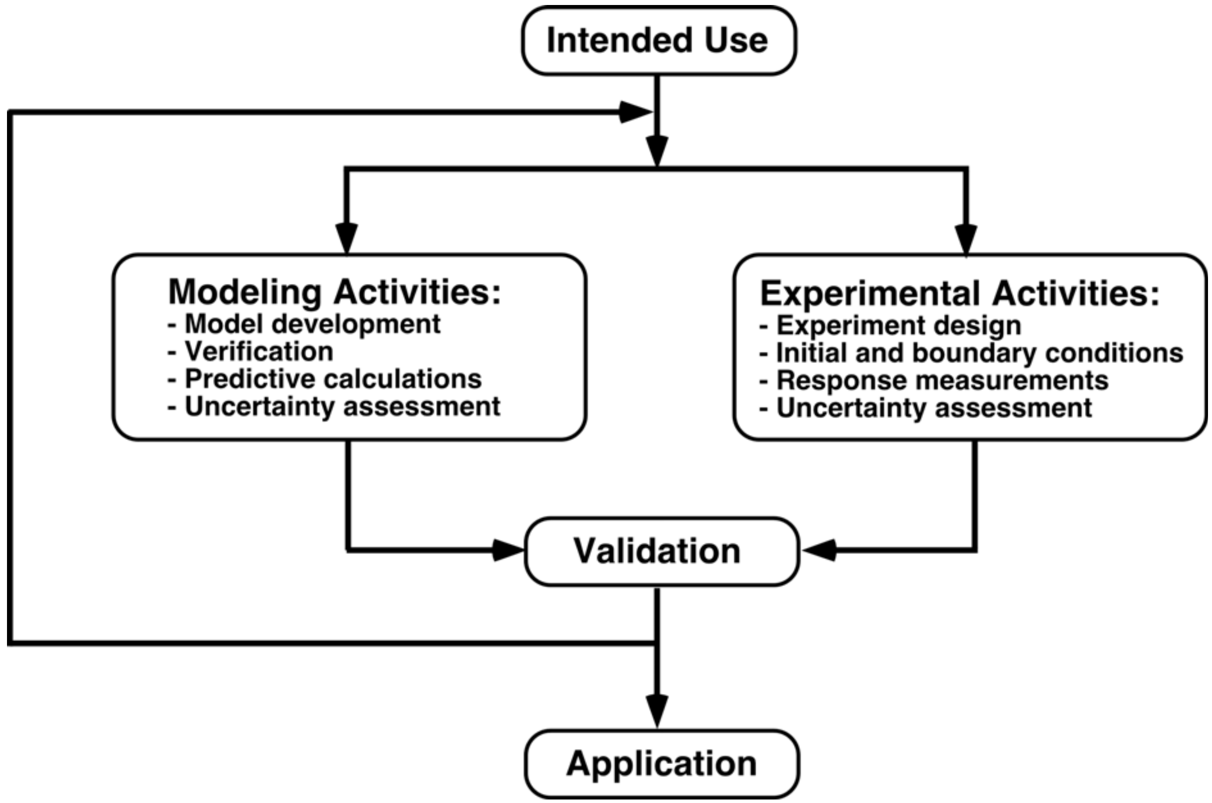
- **<u>Type 1</u>: DE estimators based on higher-order estimates of the exact solution to the PDEs (post-process the solution)**
  - **Richardson extrapolation-based methods**
  - **Order refinement methods**
  - **Finite element recovery methods (Zienkiewicz and Zhu)**
- **<u>Type 2</u>: Residual-based methods (include additional information about PDE and BCs/ICs being solved)**
  - **DE transport equations (Babuska and Rheinboldt)**
  - **Finite element residual methods (Babuska and Rheinboldt)**
  - **Adjoint methods for SRQs (Jameson, Ainsworth and Oden)**

As a minimum, one should investigate the sensitivity of the SRQs of interest to the discretization level

Formal Definition of Validation (DoD, AIAA, ASME)

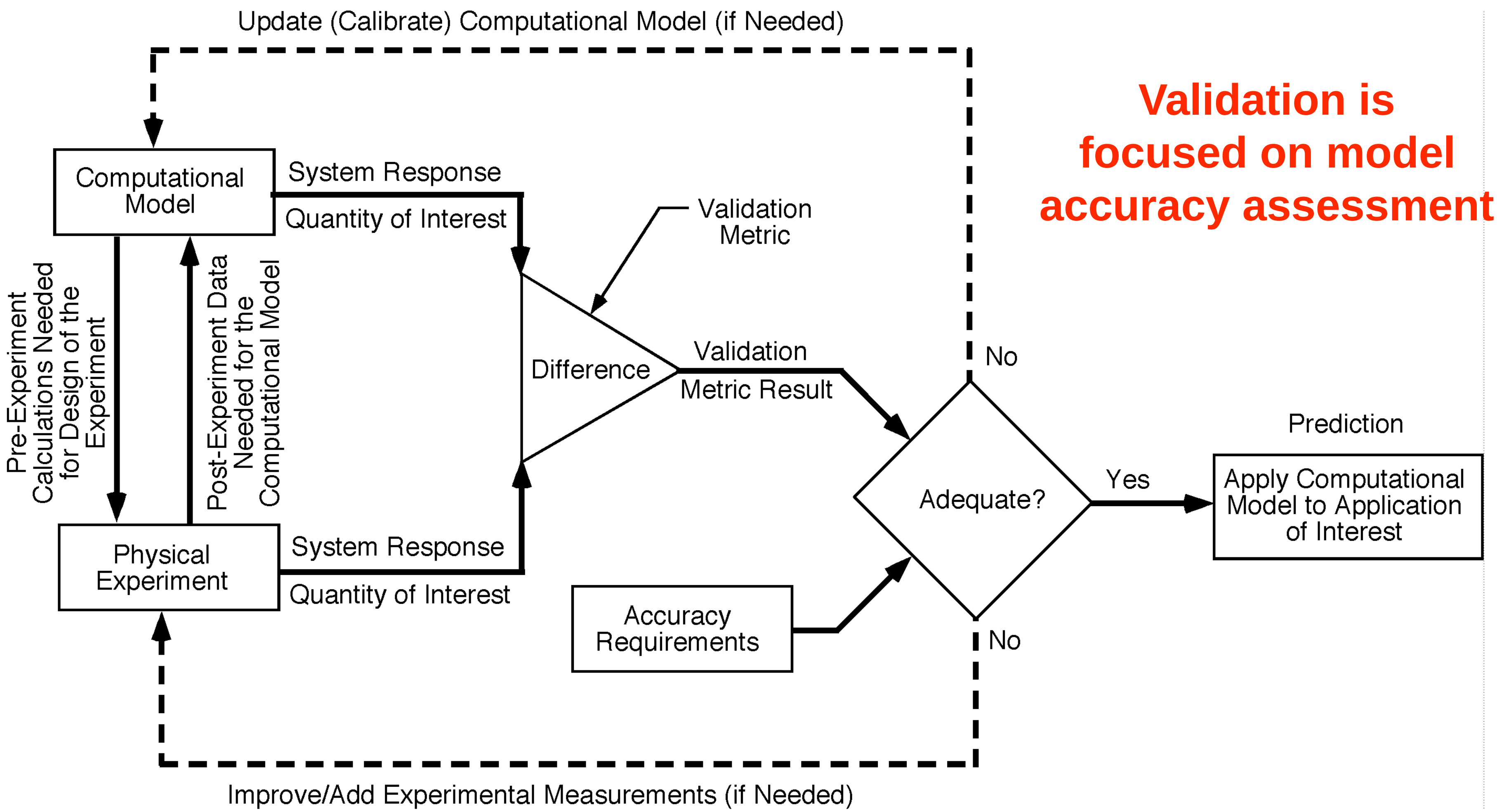
Validation: **The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.**

Validation deals with physics modeling fidelity



(Ref: ASME Guide, 2006)

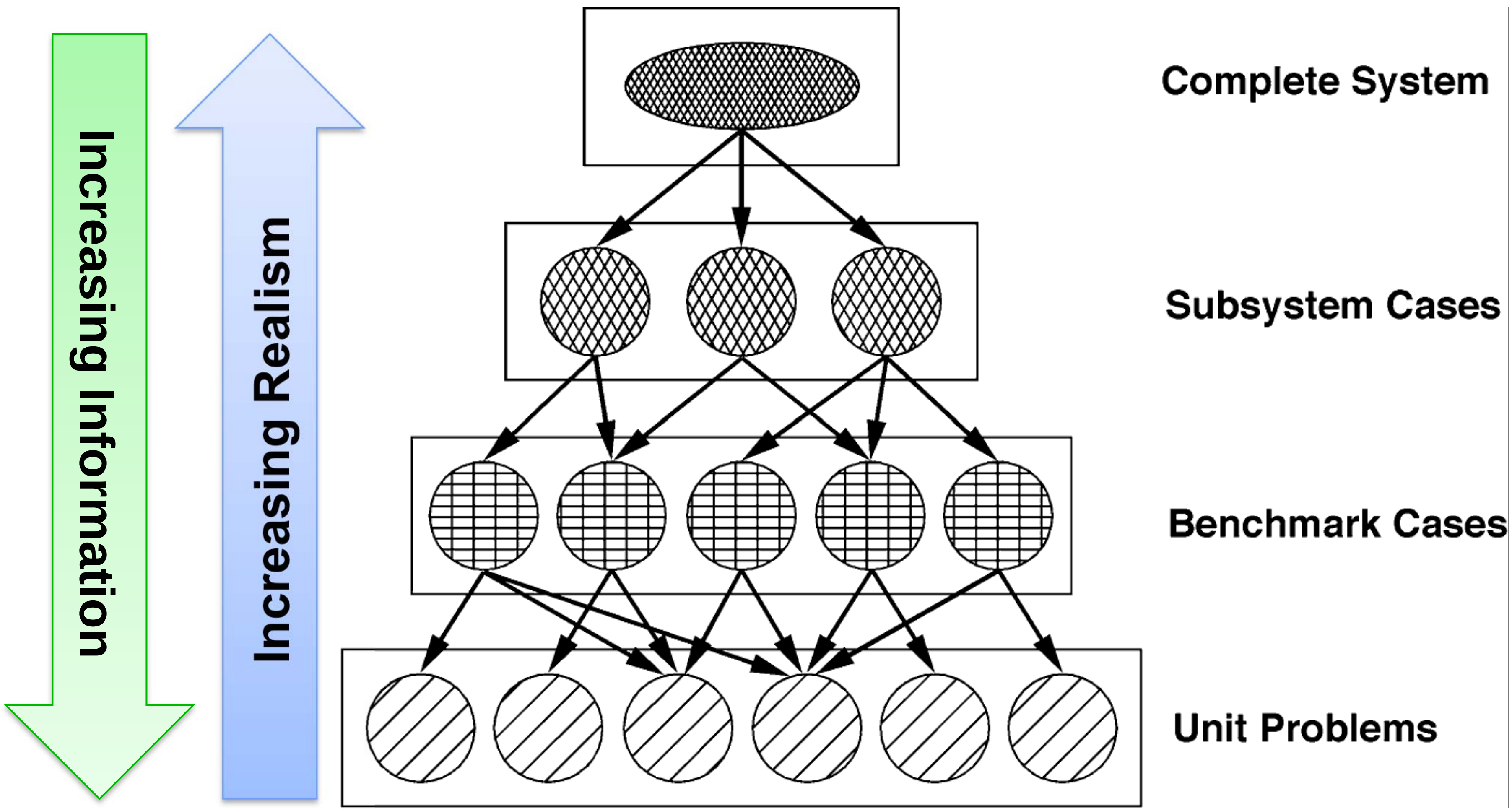
Validation, Calibration, and Prediction



Validation is focused on model accuracy assessment

(from Oberkampf and Barone, 2006)

Validation Experiment Hierarchy



(Ref: AIAA Guide, 1998)

Validation Metrics

What is a validation metric?

A quantitative measure of agreement between computational results and experimental measurements for the SRQs of interest

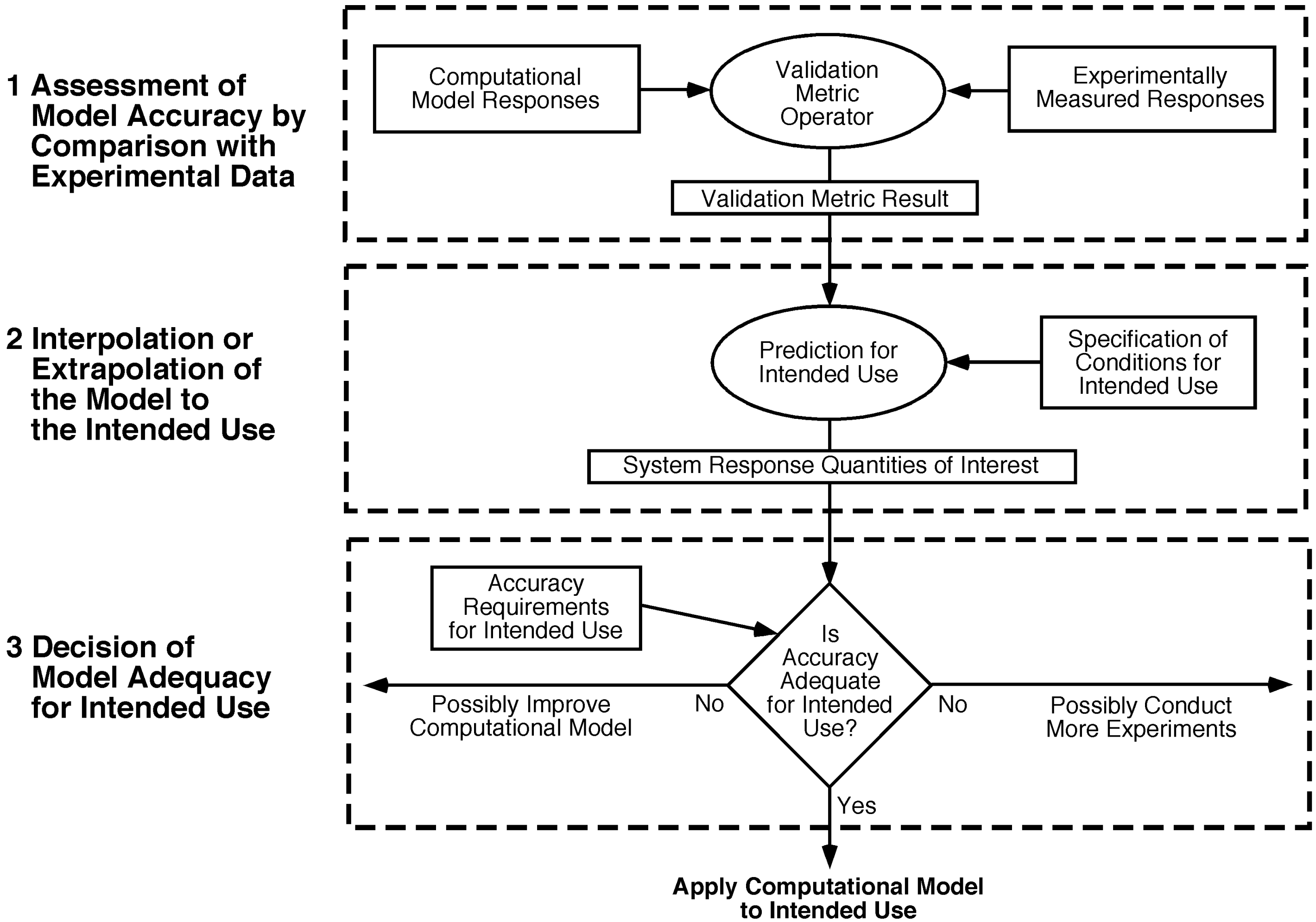
Approaches to validation metrics:

1. **Hypothesis testing methods**
2. **Comparing the statistical mean of the simulation and and the mean of the experimental measurements**
3. **Bayesian methods**
4. **Comparison of cumulative distribution functions from the simulation and the experimental measurements (area metric)**

What are the goals of using a validation metric?

- **Estimate model form uncertainty, i.e., error due to approximations and simplifications in constructing the mathematical model**

Aspects of Validation and Prediction



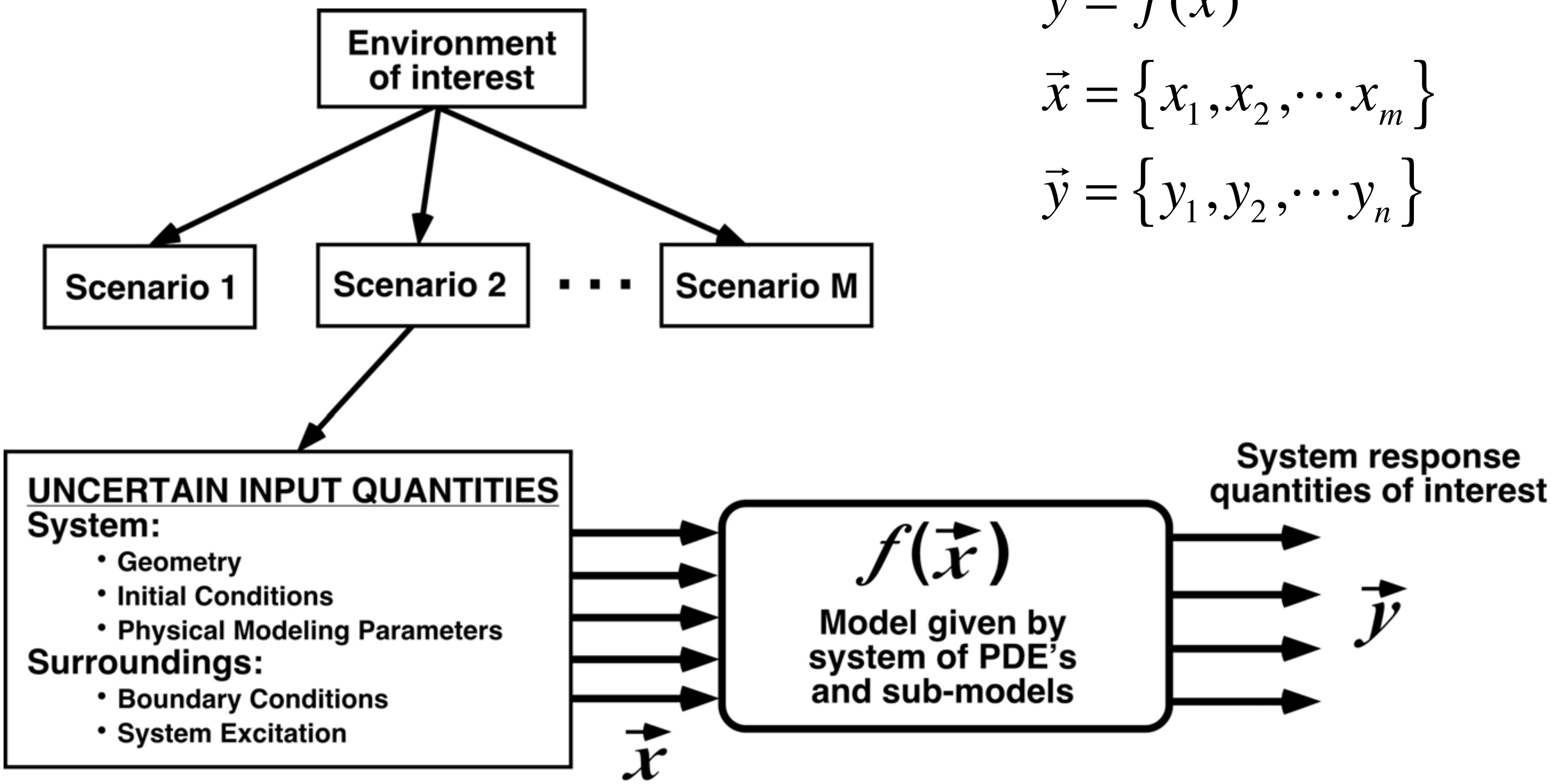
(Ref: Oberkampf and Trucano, 2008)

Predictive Capability

$$\vec{y} = f(\vec{x})$$

$$\vec{x} = \{x_1, x_2, \cdots x_m\}$$

$$\vec{y} = \{y_1, y_2, \cdots y_n\}$$

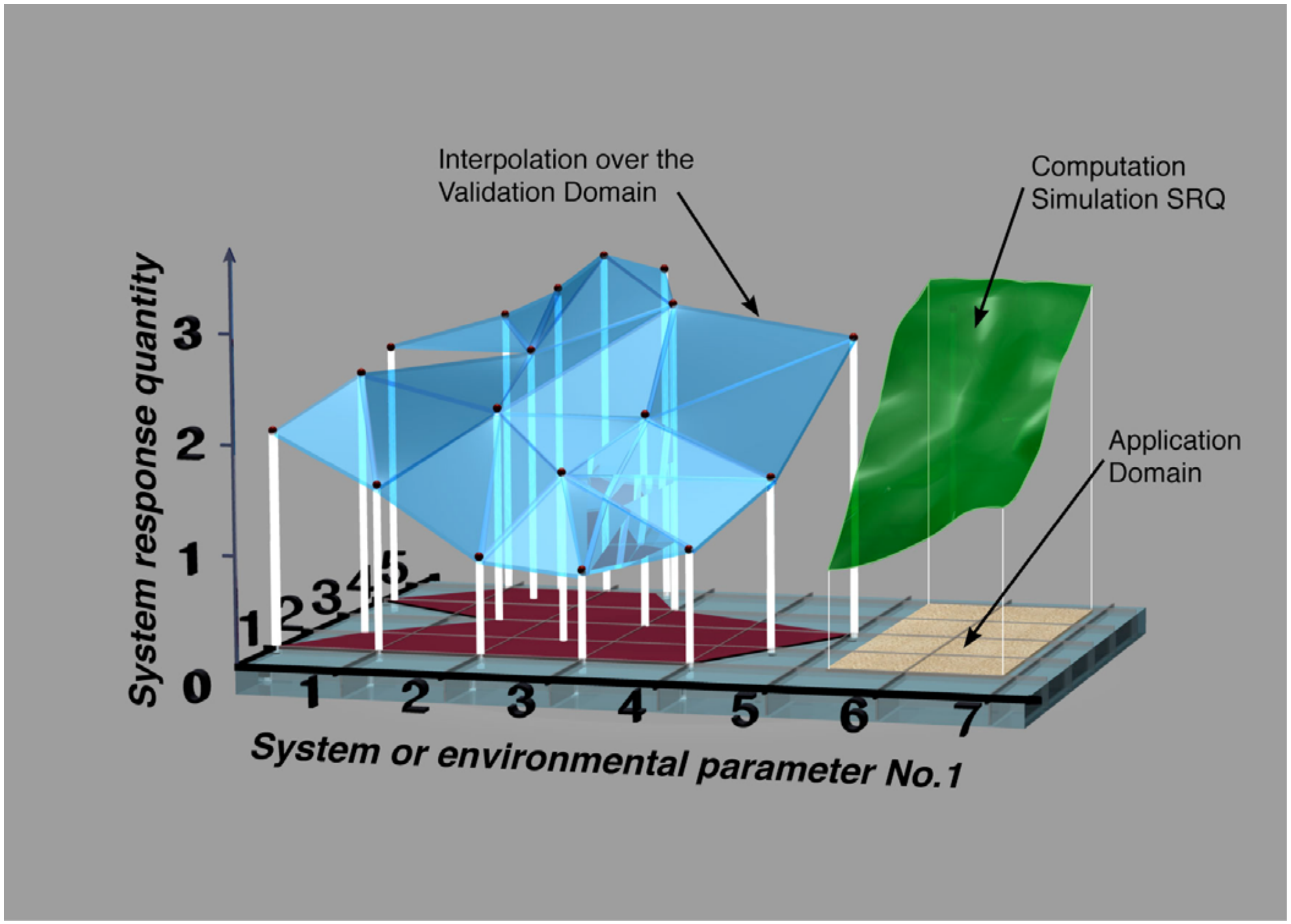


(from Oberkampf and Roy, 2010)

Sources of Uncertainty

- **Uncertainty in input parameters:**
  - Input data parameters (independently measureable and non-measureable)
  - Probability distribution parameters
  - Numerical algorithm parameters
- **Numerical solution error:**
  - Round-off error
  - Iterative error
  - Spatial, temporal, frequency discretization error
- **Model form uncertainty:**
  - Assessed over the validation domain using a validation metric
  - Extrapolated to the application conditions outside of the validation domain

Prediction Inside and Outside the Validation Domain



(from Oberkampf and Roy, 2010)

- **Extrapolations can occur in terms of:**
  - **Input quantities**
  - **Non-parametric spaces, higher tiers in the validation hierarchy**
- **Extrapolation may result in:**
  - **Large changes in coupled physics**
  - **Large changes in geometry or subsystem interactions**
- **Extrapolation should result in increases in uncertainty**

Types of Uncertainty

Aleatory uncertainty: uncertainty due to inherent randomness.

- **Also referred to as irreducible uncertainty, variability, and stochastic uncertainty**

Aleatory uncertainty is a characteristic of the system of interest

- **Examples:**
  - **Variability in neutron cross-section due to manufacturing**
  - **Variability in geometry and surface properties due to manufacturing**

Epistemic uncertainty: uncertainty due to lack of knowledge.

- **Also referred to reducible uncertainty, knowledge uncertainty, model form uncertainty, and subjective uncertainty**

Epistemic uncertainty is a characteristic of our knowledge of the system

- **Examples:**
  - **Poor understanding of physical phenomena, e.g., turbulence, coupled physics**
  - **Model form uncertainty**

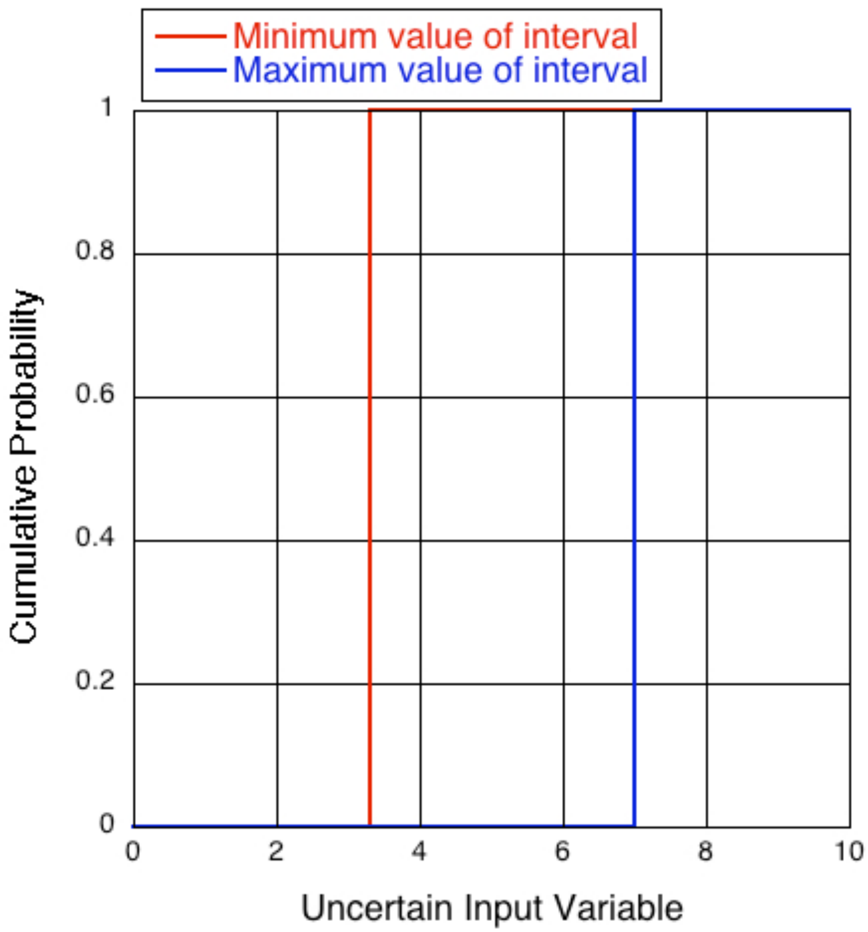
(Ref: Kaplan and Garrick, 1981; Morgan and Henrion, 1990; Ayyub and Klir, 2006)

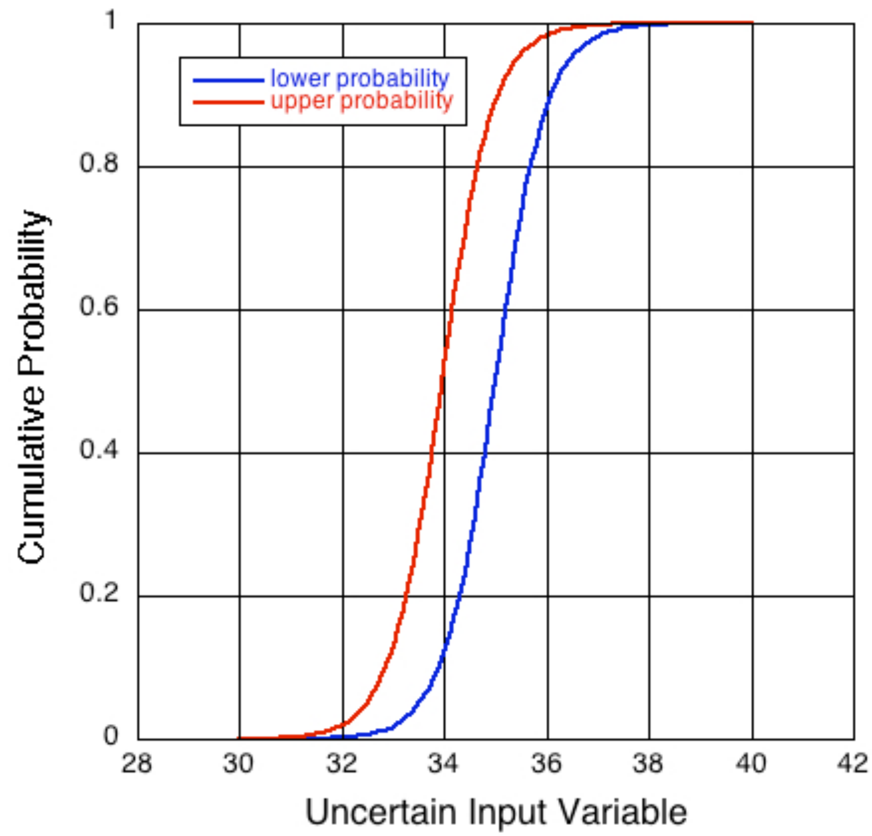
Characterization of Epistemic Uncertainty

A purely epistemic uncertainty is given by an interval (*a*,*b*)

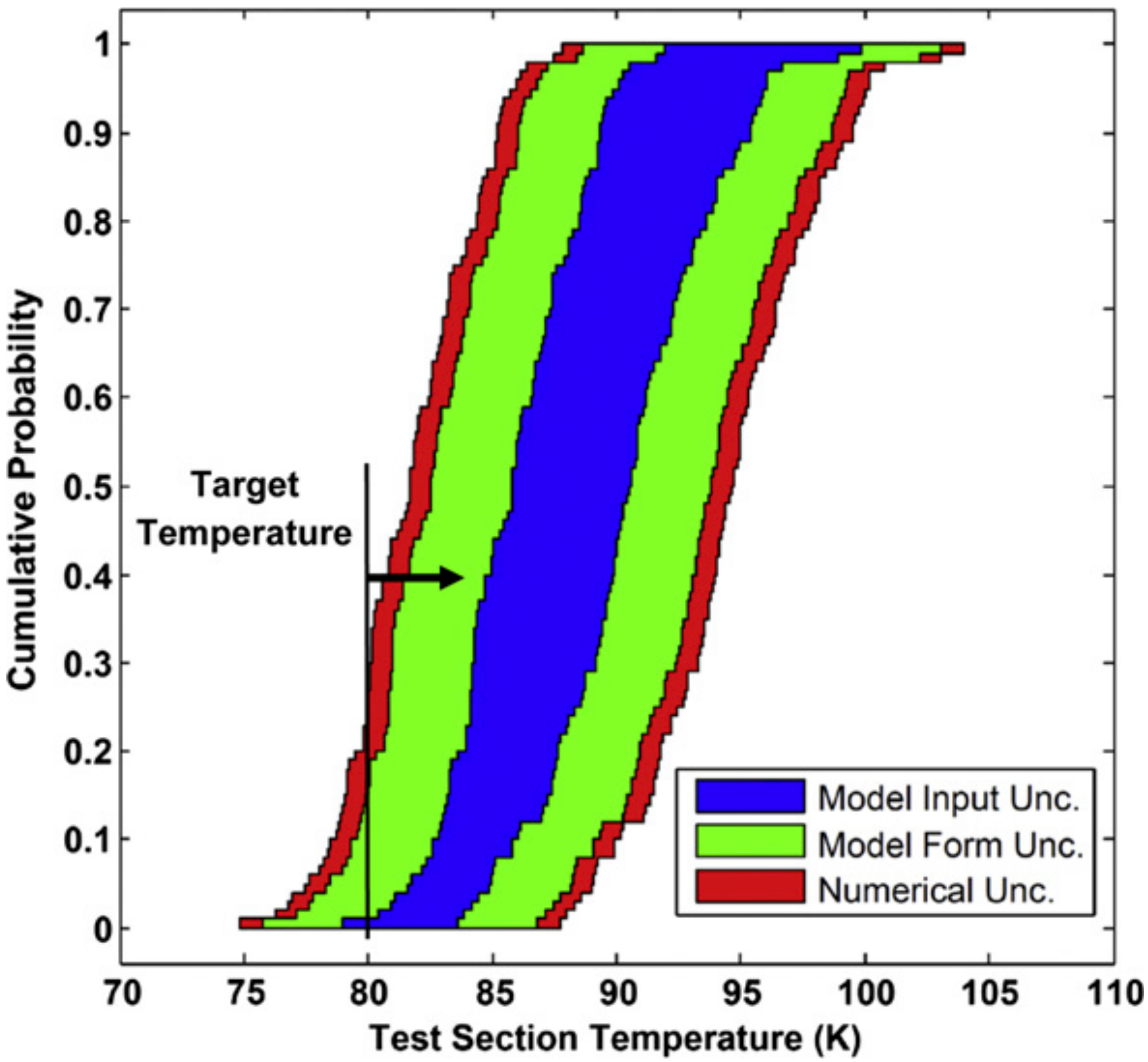
A mixture of epistemic and aleatory uncertainty is given by a p-box

This mathematical structure is referred to as an imprecise probability.





Example of Probability-box with a Mixture of Aleatory and Epistemic Uncertainty



(from Roy and Oberkampf, 2011)

Concluding Remarks

- Methodology and procedures for code and solution verification are fairly well developed, but poorly practiced
- Methodology for validation experiments has been developed
- Application of validation experiment principles have primarily been practiced in computational fluid dynamics
- Verification and validation are focused on assessment
- Prediction is focused on what we have never seen before
- Explicitly including all of the sources of uncertainty in a prediction are not always welcomed

VVUQ are focused on truth in simulation, not marketing

Some Prefer to Take the Position

"I don't have the time, money, or people to do VVUQ."

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