Verification, Validation, and Predictive Capability: What's What?

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Outline

- Motivation and background
- Code and solution verification
- Model validation and calibration
- Predictive capability
- Closing remarks

Motivation

- We are in the midst of a revolution in science and engineering
- Impact of modeling and simulation are dramatically increasing in geophysical systems because:
  - Traditional experiments for the understanding of systems are usually impossible
  - Large physical scales and long time spans make simulation most appealing
  - Ability to optimize and perturb our designs in unique ways
  - Stunning reduction in cost of computing resources

How can simulation analysts and customers who use simulations determine if the simulation results can be trusted?

Background

- What elements determine if suppliers and customers can trust simulation results?
  - Education and training of the computational analysts
  - Development and implementation of quality control processes for simulation activities, e.g., simulation governance
  - Use of verification and validation procedures
  - Estimation of the uncertainties that could impact the results
- There are different types of verification and validation:
  - System V&V
  - Software V&V
  - Simulation V&V
- All have similar concepts:
  - Verification: Am I building the product correctly?
  - Validation: Am I building the correct product?

We will focus on simulation V&V and predictive capability

Conceptual Framework of Simulation Verification, Validation and Predictive Capability

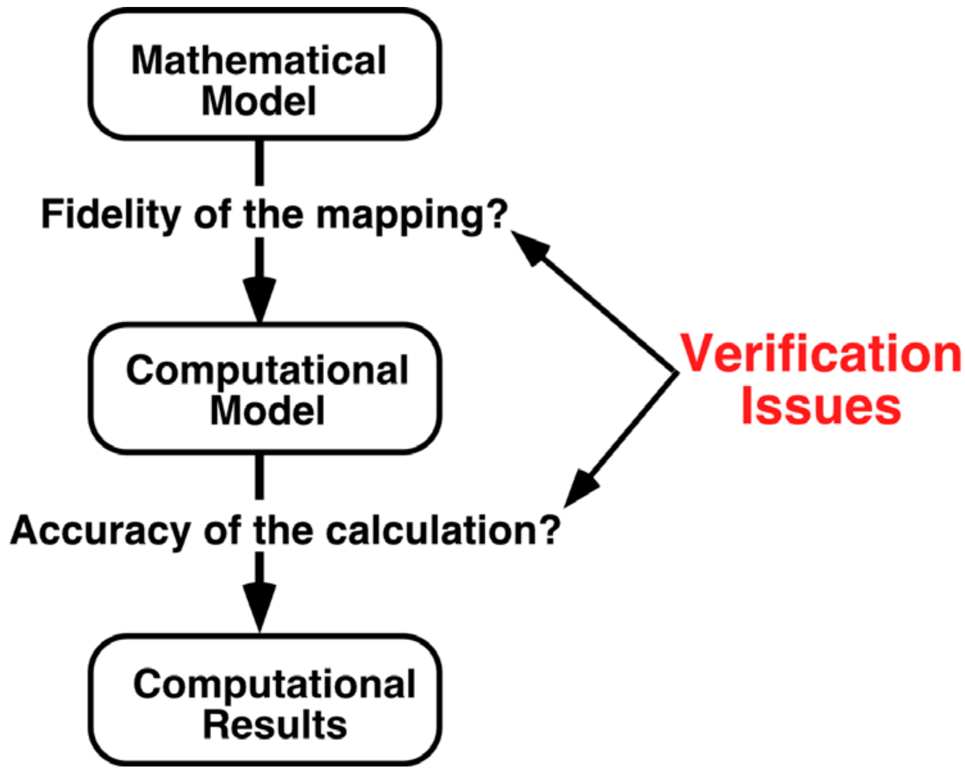
- **Verification and validation are built on the philosophy of skepticism**
  - **The fundamental procedure of V&V is testing**
  - **"Show me the evidence that the software and the mathematical models are working properly."**
- **Predictive capability is foretelling the state of the system for conditions where no experimental data are available:**
  - **Predictive capability is built on:**
    - **Fidelity of the physics modeling embodied in the mathematical model**
    - **Identification and estimation of all sources of uncertainty for the system conditions of interest**
  - **The procedure is built on uncertainty quantification (UQ) using non-deterministic simulation**

Predictive capability is the primary reason for conducting simulation

Formal Definition of Verification (U.S. DoD, AIAA, ASME, ASCE)

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

Verification assesses software reliability and numerical accuracy



Two Types of Verification
First: Code Verification

- **Code verification activities are directed toward:**
  - **Finding and removing mistakes in the source code**
  - **Finding and removing errors in the numerical algorithms**

  Primary Result: determination of the observed order of numerical convergence in space and time

- **Responsibility for code verification activities:**
  - **Primary: software developers (either commercial or developers within an organization)**
  - **Secondary: simulation analysts (customers of software developers) and customers of the simulation**

- **Status of code verification:**
  - **Commercial software: very few (if any) document the observed order of accuracy of their solutions**
  - **Organizational software: very few organizations document the observed order of accuracy of their solutions**

Two Types of Verification
Second: Solution Verification

- Solution verification activities are directed toward:
  - Assuring the correctness of input and output data for each problem of interest
  - Estimating the numerical solution error
- Sources of numerical solution error:
  - Round-off error
  - Iterative error
  - Discretization error
  - Statistical sampling error
  - Response surface error

Primary Goal: Estimation of the total numerical solution error in the system response quantities (SRQs) of interest

Solution Verification (continued)

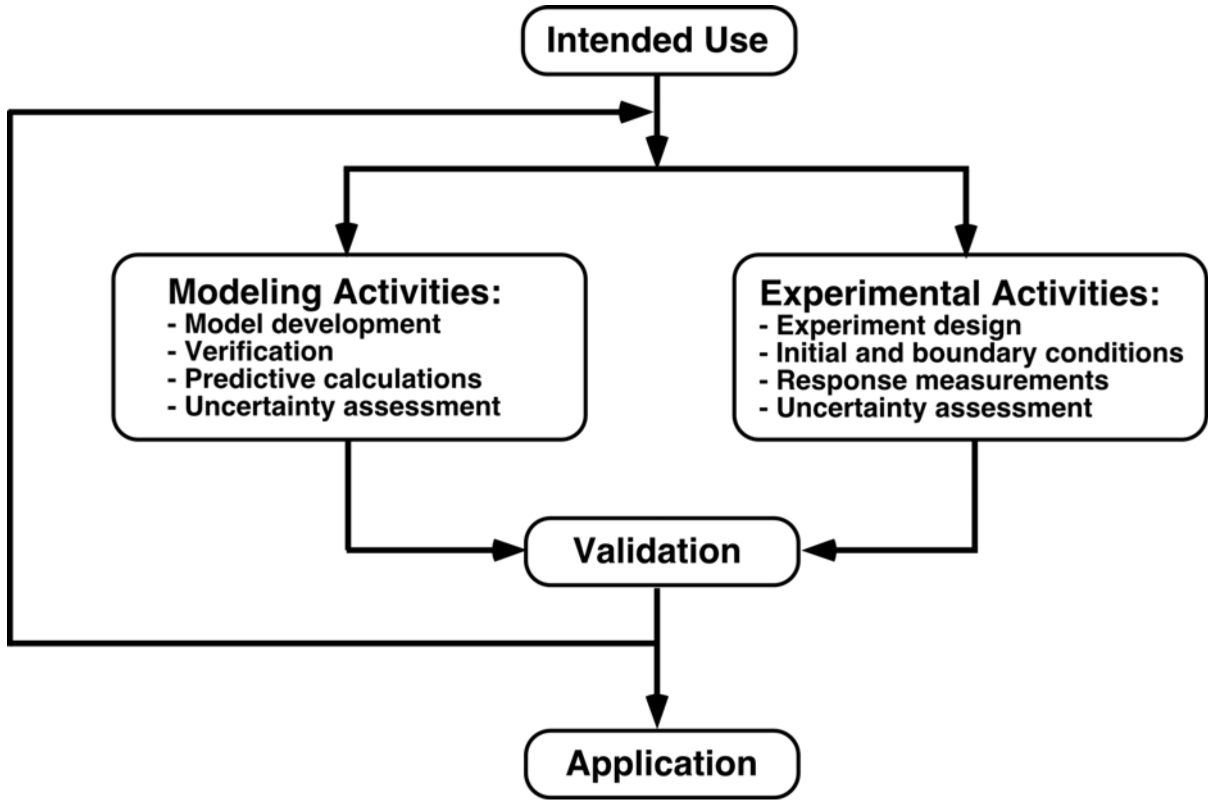
- Classification of discretization error estimators:
  - Type 1: DE estimators based on higher-order estimates of the exact solution to the PDEs (Richardson extrapolation, order refinement methods, and finite element recovery methods)
  - Type 2: DE estimator based on estimating the discretization residual of the PDEs (DE transport equation method, finite element residual methods, and adjoint methods)
- Responsibility for solution verification:
  - Primary: simulation analysts
  - Secondary: software developers (for implementing estimation tools) and customers of the simulation
- Status of solution verification:
  - Very few analysts estimate solution error
  - Very few managers/decision makers ask about solution verification

"But our results agree with the experimental data."

Formal Definition of Validation (U.S. DoD, AIAA, ASME, ASCE)

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

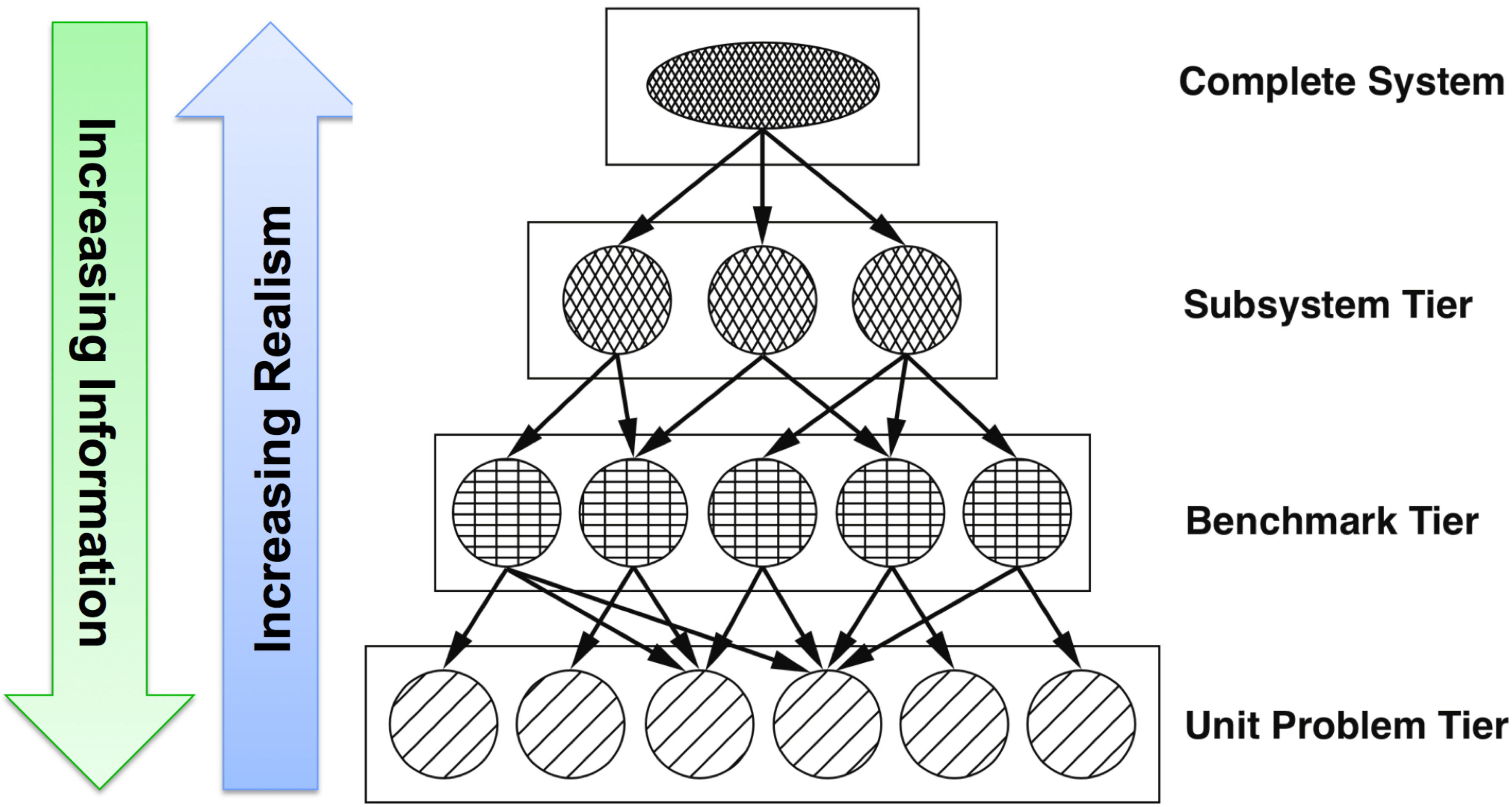


(Ref: ASME Guide, 2006)

Goals and Tools of Validation

- **Tactical goals of validation:**
  - **Quantification of the effects of mathematical modeling assumptions and approximations by comparison of simulation results with experimental measurements, i.e., quantification of model form uncertainty**
  - **Quantification of model form uncertain (distinct from parametric uncertainty)**
- **Strategic goals of validation:**
  - **Improve mathematical modeling to increase predictive capability**
  - **Improve the separation of model form uncertainty from input parameter uncertainty**
- **What are the primary tools of validation?**
  - **High quality validation experiments**
  - **Validation metrics: mathematical operators to quantify the difference between simulation and experimental outcomes**

Validation Experiment Hierarchy for Engineering Systems



(Ref: AIAA Guide, 1998)

Model Calibration

Calibration: (AIAA and ASME definition) The process of adjusting physical modeling parameters in the computational model to improve agreement with experimental data

- Also known as: parameter estimation, model tuning, model updating
- Calibration is commonly conducted **before** formal validation activities
- Ex: Calibration of erosion parameters, calibration of subsurface porosity and permeability, and calibration of chemical and biological parameters

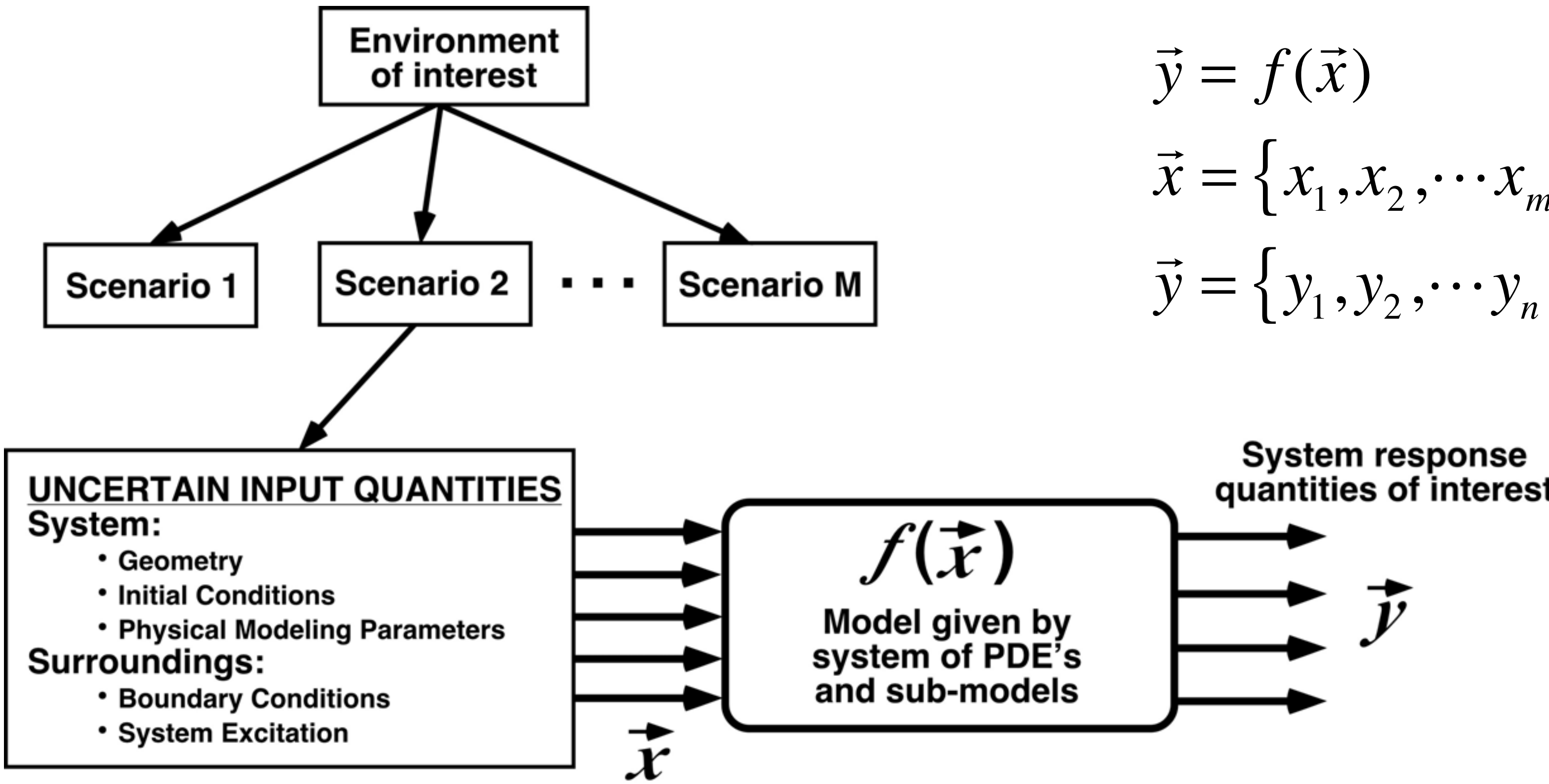
Approaches to model calibration:

- Frequentist (classical) approaches
- Bayesian updating:
  - Parameters are considered as probability distributions
  - Probability distributions represent belief likelihoods
  - Parameters are updated using Bayes formula when new experimental data become available

Where Do We Stand: Validation Activities

- **Common approach to validation is actually model calibration:**
  - **Parameters in the model, either scalars or probability distributions, are adjusted to improve agreement with experimental data**
  - **Simulations are usually reliable when the models are used for very similar systems and conditions for which the models are calibrated**
  - **Weaknesses in the models are not uncovered, but masked, when model calibration becomes dominant**
- **To improve confidence in our simulations, validation should:**
  - **Improve the separation of calibration and validation activities**
  - **Emphasize the assessment of simulation accuracy by using blind-predictions of experimental data**
  - **Improve cooperation and synergism between experimentalists and computational analysts**

Predictive Capability: Reliance on Non-Deterministic Simulations



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

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

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

- **Key sources of uncertainty:**
  - **Identification of environments and scenarios that the system could experience**
  - **Input uncertainties in the system and in the surroundings**
  - **Model form uncertainty, i.e., uncertainty in** $f(\vec{x})$
  - **Numerical errors in** $\vec{y}$

Types of Uncertainties

Aleatory uncertainty: uncertainty due to inherent randomness

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

  Aleatory uncertainty is a characteristic of the system of interest

- **Examples:**
  - **Variability weather conditions, e.g., wind speed, rain fall, temperature**
  - **Variability in properties of natural and manmade materials**
  - **Variability in excitation, e.g., frequency and amplitude of earthquakes**

Epistemic uncertainty: uncertainty due to lack of knowledge

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

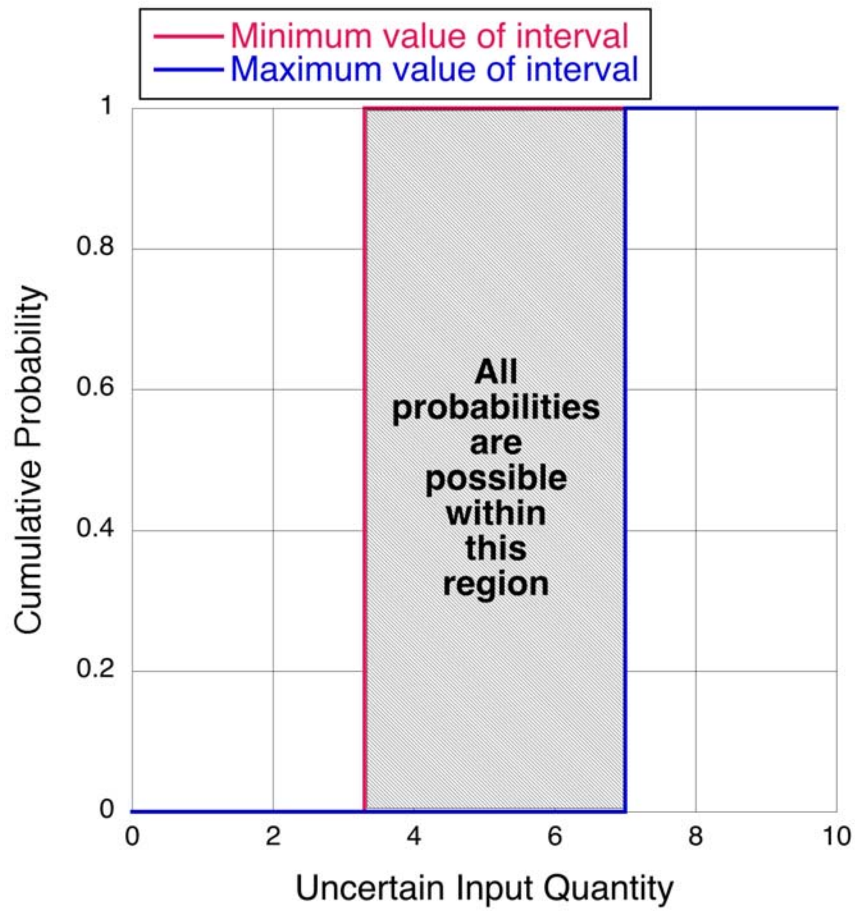
  Epistemic uncertainty is a characteristic of our knowledge of the system

- **Examples:**
  - **Poor understanding of physical phenomena, e.g., underground transport**
  - **Poor understanding of accident scenarios and event/failure trees**
  - **Model form uncertainty, e.g., failure of large man-made structures**

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

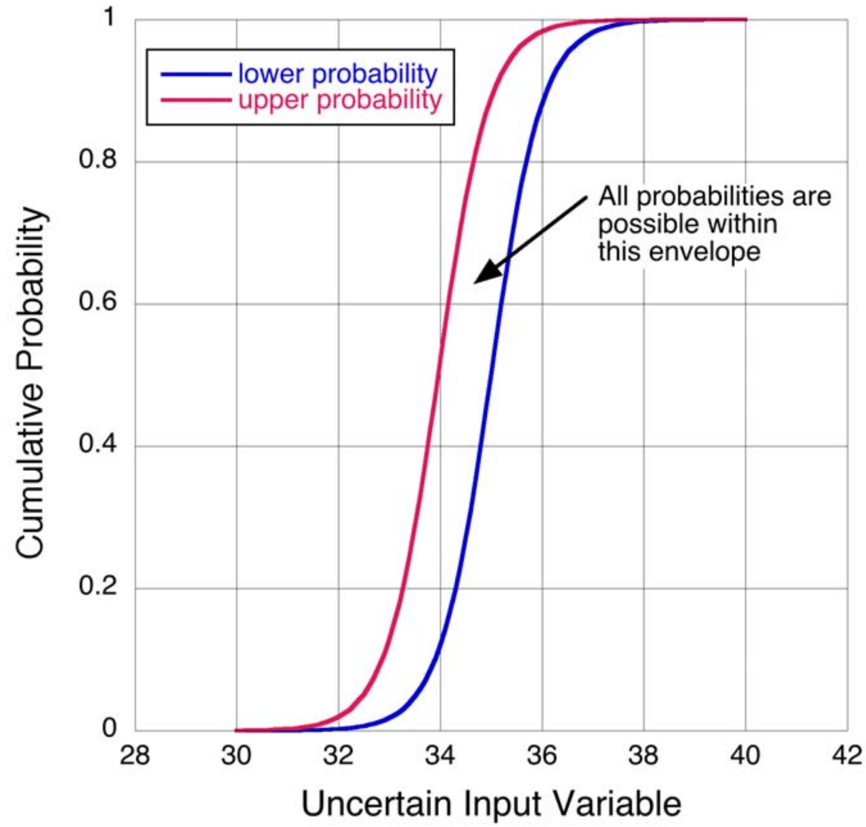
Characterization of Epistemic Uncertainty

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

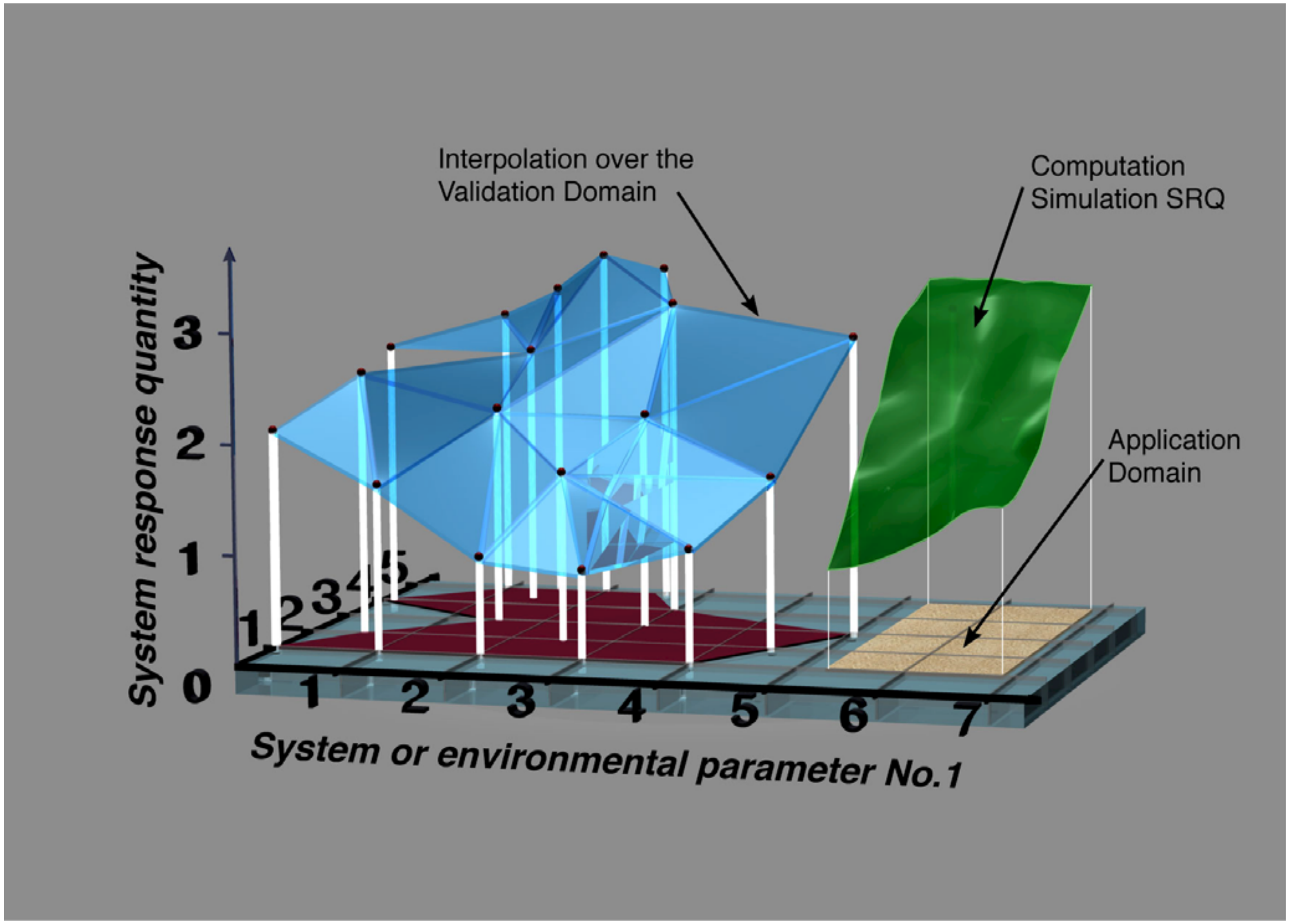


A mixture of epistemic and aleatory uncertainty is characterized by a p-box

This mathematical structure is referred to as an imprecise probability.



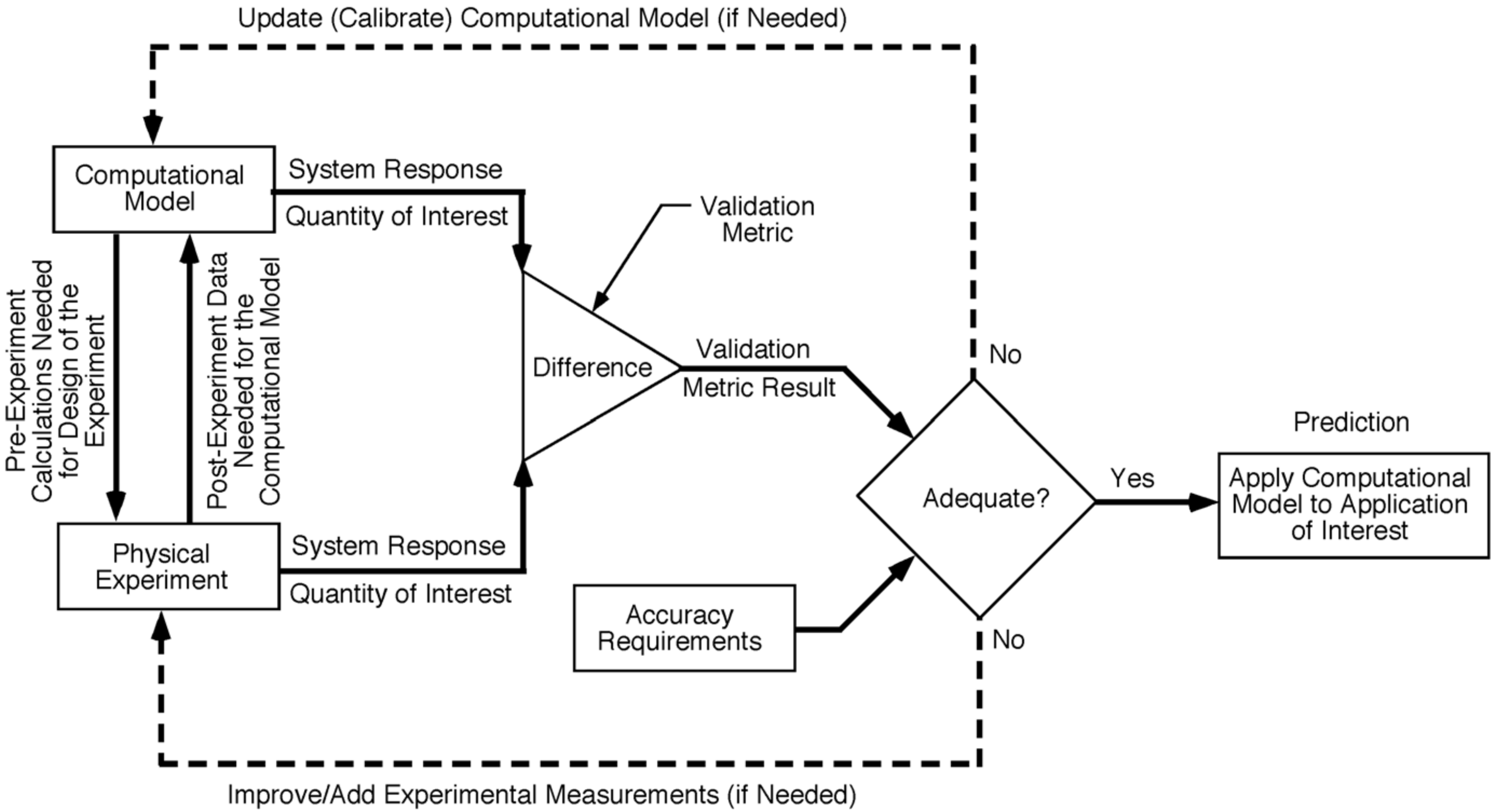
Prediction Far From the Validation/Calibration Domain: Extrapolation



(Ref: Oberkampf and Roy, 2010)

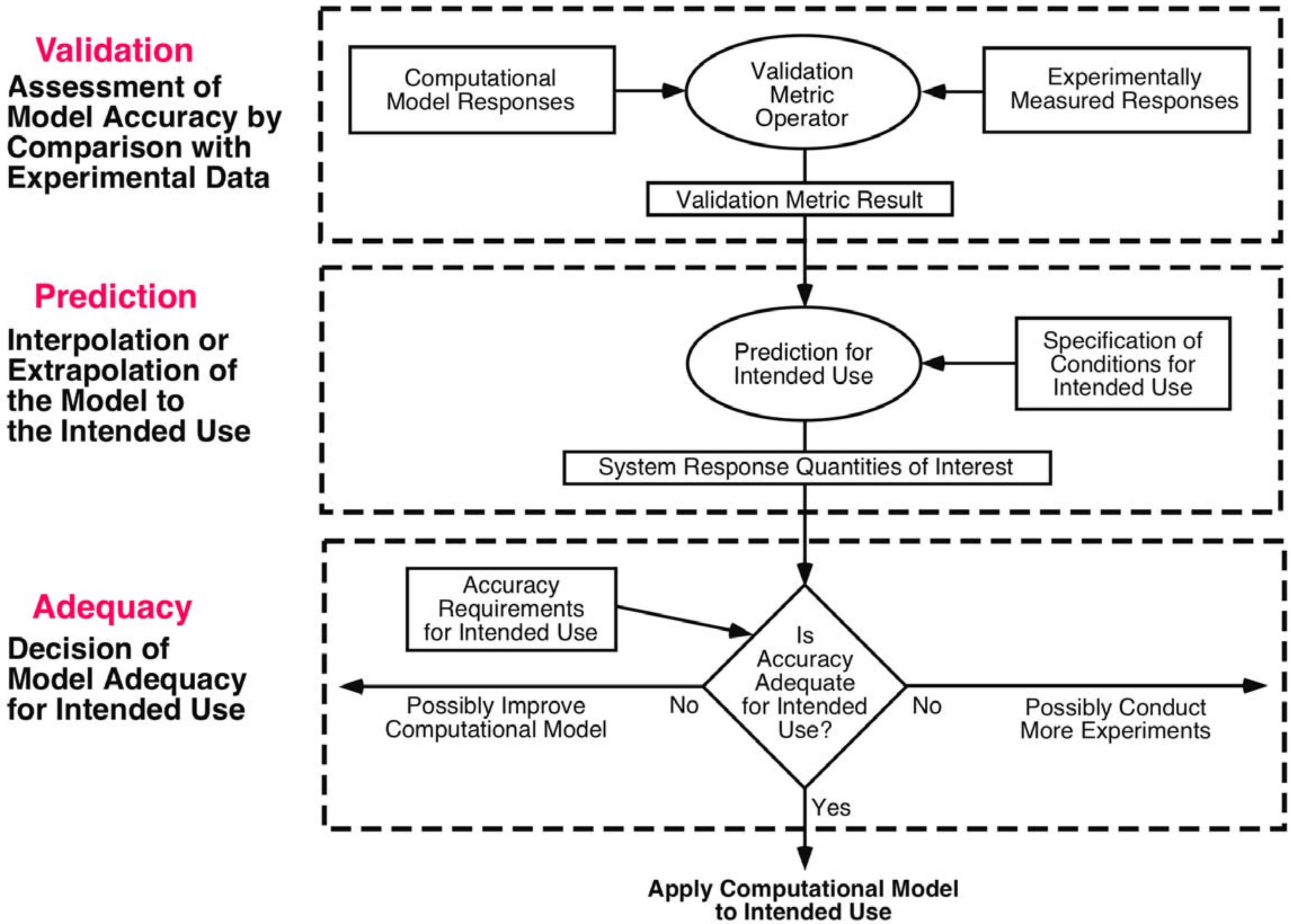
- **Extrapolation can occur in terms of:**
  - **Input parameters**
  - **Higher levels in the validation hierarchy**
- **Large extrapolations commonly involve large changes in physics coupling**
- **Large extrapolations should be based on physics inference, not statistical inference**

Validation (Model Accuracy) Assessment, Calibration and Prediction



(Ref: Oberkampf and Barone, 2006)

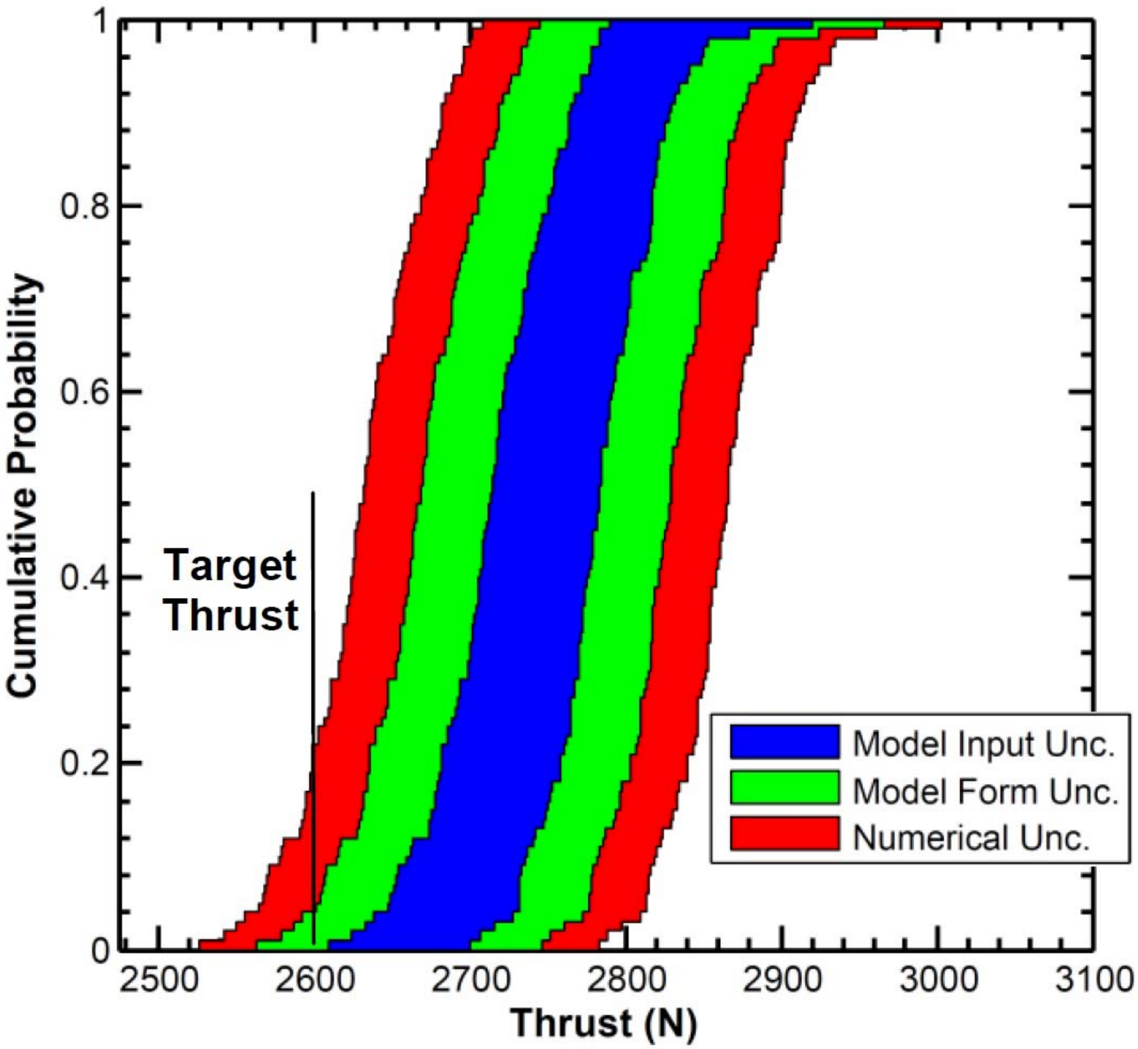
Contrasting Validation, Prediction, and Model Adequacy



(Ref: Oberkampf and Trucano, 2008)

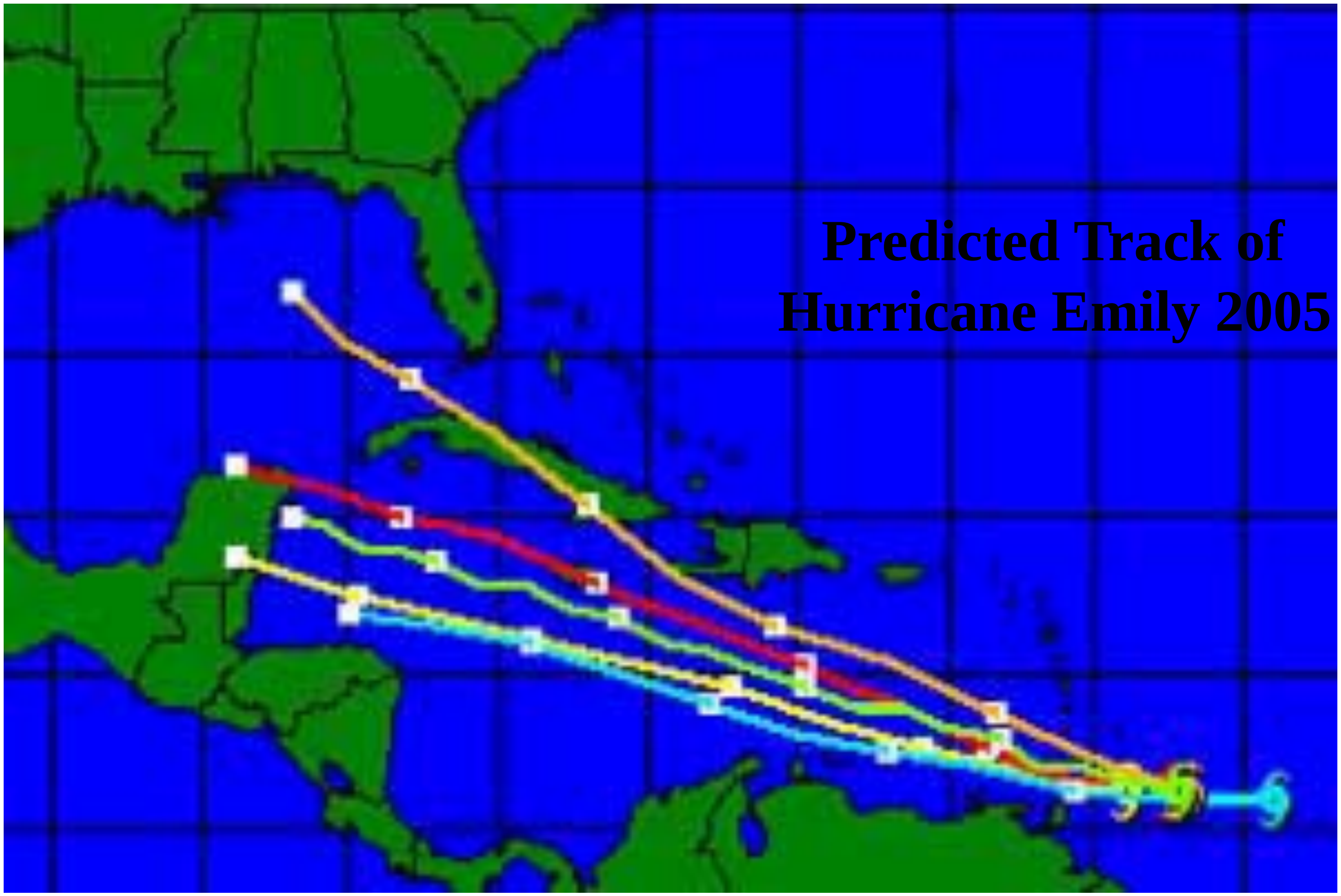
Example of a Probability-Box with Various Sources of Uncertainty

(Roy and Balch, 2012)



- **Prediction of thrust from a small rocket motor**
- **Uncertain inputs to the mathematical model:**
  - **Total pressure in the motor ~ normal distribution**
  - **Effect of boundary layer transition ~ interval-valued effect on the expansion ratio of the nozzle**
- **Epistemic uncertainties in the simulation are:**
  - **Model form uncertainty**
  - **Numerical solution error**

Example Showing Total Uncertainty Using Alternate Competing Models



(Ref: Green, 2007)

Closing Remarks

- **Code and solution verification must be improved to ensure we are building on a solid foundation for simulation**
- **Validation is focused on assessing the accuracy of mathematical models vis-à-vis experimental measurements**
- **In geosciences mathematical models are dominated by calibration procedures for model parameters**
- **Predictive capability:**
  - **Is focused on what we have never seen before**
  - **When we make predictions far from our validation/calibration database, we should concentrate on capturing total uncertainty**

Quote from William H. Press (author of *Numerical Recipes*):

"Simulation and mathematical modeling will power the 21st Century the way steam powered the 19th."

References

- **AIAA. (1998). "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations." American Institute of Aeronautics and Astronautics, AIAA-G-077-1998, Reston, VA.**
- **Anderson, M. G. and P. D. Bates, Eds. (2001). Model Validation: Perspectives in Hydrological Science. New York, NY, John Wiley & Sons LTD.**
- **ASME (2006), "Guide for Verification and Validation in Computational Solid Mechanics," American Society of Mechanical Engineers, ASME V&V 10-2006.**
- **ASME (2012), "An Illustration of the Concepts of Verification and Validation Computational Solid Mechanics," American Society of Mechanical Engineers, ASME V&V 10.1-2012.**
- **Ayyub, B. M. and G. J. Klir (2006). Uncertainty Modeling and Analysis in Engineering and the Sciences, Boca Raton, FL, Chapman & Hall.**
- **DoD (2000), Verification, Validation, and Accreditation (VV&A) Recommended Practices Guide, Department of Defense Modeling and Simulation Coordination Office, www.msco.mil**
- **Ferson, S., W. L. Oberkampf, and L. Ginzburg (2008), "Model Validation and Predictive Capability for the Thermal Challenge Problem," *Computer Methods in Applied Mechanics and Engineering*, Vol. 197, pp. 2408-2430.**
- **Haimes, Y. Y. (2009), Risk Modeling, Assessment, and Management, 3rd edition, New York, John Wiley.**
- **Oberkampf, W. L. and T. G. Trucano (2002), "Verification and Validation in Computational Fluid Dynamics," *Progress in Aerospace Sciences*, Vol. 38, No. 3, pp. 209-272.**

References (continued)

- Oberkampf, W. L., T. G. Trucano, and C. Hirsch (2004), “Verification, Validation, and Predictive Capability,” *Applied Mechanics Reviews*, Vol. 57, No. 5, pp. 345-384.
- Oberkampf, W. L. and M. F. Barone (2006), "Measures of Agreement Between Computation and Experiment: Validation Metrics," *Journal of Computational Physics*, Vol. 217, No. 1, pp. 5-36.
- Oberkampf, W. L. and T. G. Trucano (2008), “Verification and Validation Benchmarks,” *Nuclear Engineering and Design*, Vol. 238, No. 3, 716-743.
- Oberkampf, W.L. and C. J. Roy (2010), <u>Verification and Validation in Scientific Computing</u>, Cambridge University Press, Cambridge, UK.
- Roy, C. J. (2005). "Review of Code and Solution Verification Procedures for Computational Simulation." *Journal of Computational Physics. 205(1), 131-156.*
- Roy, C. J. and W. L. Oberkampf (2011). "A Comprehensive Framework for Verification, Validation, and Uncertainty Quantification in Scientific Computing." *Computer Methods in Applied Mechanics and Engineering. 200(25-28), 2131-2144.*
- Szabo, B. and R. Actis (2012). "Simulation Governance: Technical Requirements for Mechanical Design." *Computer Methods in Applied Mechanics and Engineering. 249-252, 158-168.*
- Trucano, T. G., L. P. Swiler, T. Igusa, W. L. Oberkampf and M. Pilch (2006). "Calibration, Validation, and Sensitivity Analysis: What's What." *Reliability Engineering and System Safety. 91(10-11), 1331-1357.*
- Vose, D. (2008). <u>Risk Analysis: A quantitative guide. 3rd Ed., New York, Wiley.</u>