Development and Use of Engineering Standards for Computational Fluid Dynamics for Complex Aerospace Systems

AIAA Committee on Standards in CFD
Hyung Lee
Urmila Ghia
Sami Bayyuk
William L. Oberkampf
Christopher J. Roy
John A. Benek
Christopher L. Rumsey
Joseph M. Powers
Robert H. Bush
Mortaza Mani

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AIAA Guide for Verification and Validation of Computational Fluid Dynamics Simulations

- AIAA Guide (AIAA G-077), originally published in 1998, was the first engineering standards document available to engineering community for verification and validation (V&V) of simulations.
- AIAA Committee on Standards in CFD is currently updating the AIAA Guide to describe the V&V concepts, methods, and practices in the broader context of predictive capability and uncertainty quantification (UQ)
- The goal of the updated AIAA Guide (Guide Update) is to provide a foundation for understanding and addressing major issues and concepts in predictive CFD.
- In practice, it is envisioned that the AIAA Guide Update will educate and inform software and methods developers, analysts, technical management and decision-makers on the value of and the need to conduct V&V and UQ for modeling and simulation.

Motivation

- Modeling and simulation (M&S) are rapidly increasing because of:
  - Reduced design time and time to new product introduction
  - Stunning reduction in cost of computing resources, including cloud computing
  - Increasing access to M&S – M&S delivered as a service
  - Ability to optimize our systems for a wide range of operating conditions
  - Ability of simulation to reduce required tests for certification
  - Reliance on simulation when testing is not possible
- We are in the midst of a revolution in practice of engineering:
  - M&S are increasingly relied on for predictive performance, reliability and safety of engineering systems.
  - Analysts, designers, project managers, decision makers, who must depend on simulation, need practical techniques and methods for assessing simulation credibility

How can we determine if the simulation results can be trusted?

Background

- How can one determine if simulation results can be trusted?
  - Education and training of the technical staff
  - Development and implementation of quality control process for simulation activities, e.g., simulation governance
  - Use of verification and validation (V&V) and uncertainty quantification (UQ) procedures
- 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?

In the AIAA Guide Update and this presentation, we will focus on Simulation V&V, UQ and Predictive Capability

Conceptual Framework of Simulation Verification, Validation and Predictive Capability

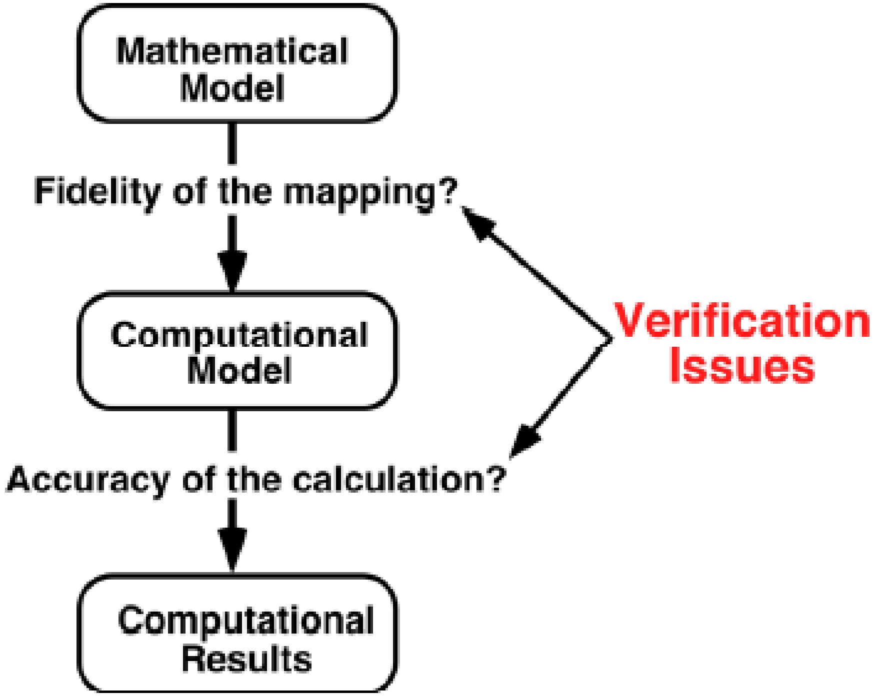
- Verification and validation are built on the philosophy of skepticism
  - The fundamental procedure of V&V is testing
  - Gathering of the evidence to show that the software and the mathematical models are working properly
- Predictive capability is foretelling the state of the system for conditions where no experimental data are available:
  - The approach is built on:
    - The fidelity of the physics modeling embodied in the mathematical model
    - The identification and estimation of all sources of uncertainty for the system conditions of interest
  - The procedure is built on uncertainty quantification using non-deterministic simulation

Predictive Capability is the primary reason for 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: Code Verification

- Code verification activities are directed toward:
  - Finding and removing errors 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, whether commercial or within an organization
  - Secondary: simulation analysts, i.e., customers of software developers
- Status of code verification
  - Commercial software: very few (if any) document the observed order of accuracy of their solutions
  - Organizational software: some organizations document the observed order of accuracy of their solutions

Two Types of Verification: Solution Verification

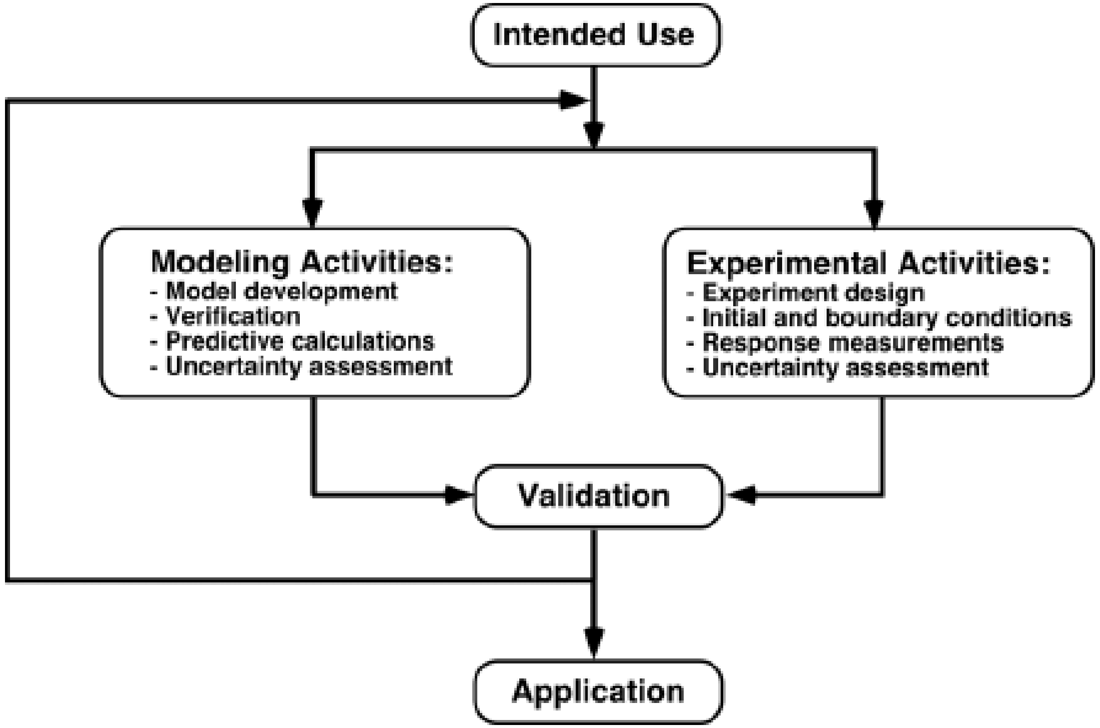
- Solution verification activities are directed toward:
  - Assuring the correctness of input and output data for the problem of interest
  - Estimating the numerical solution error caused by iteration, discretization, statistical sampling, response surface, etc.

  Primary Result: estimation of the discretization error in system response quantities (SRQs) of interest
- Responsibility for solution verification activities:
  - Primary: simulation analysts
  - Secondary: software developers (for implementing estimation tools)
- Status of solution verification
  - Very few analysts estimate solution error
  - Very few managers/decision makers ask about solution verification

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 use of the model.

Validation deals with physics modeling fidelity



Intended Use

Modeling Activities:
- Model development
- Verification
- Predictive calculations
- Uncertainty assessment

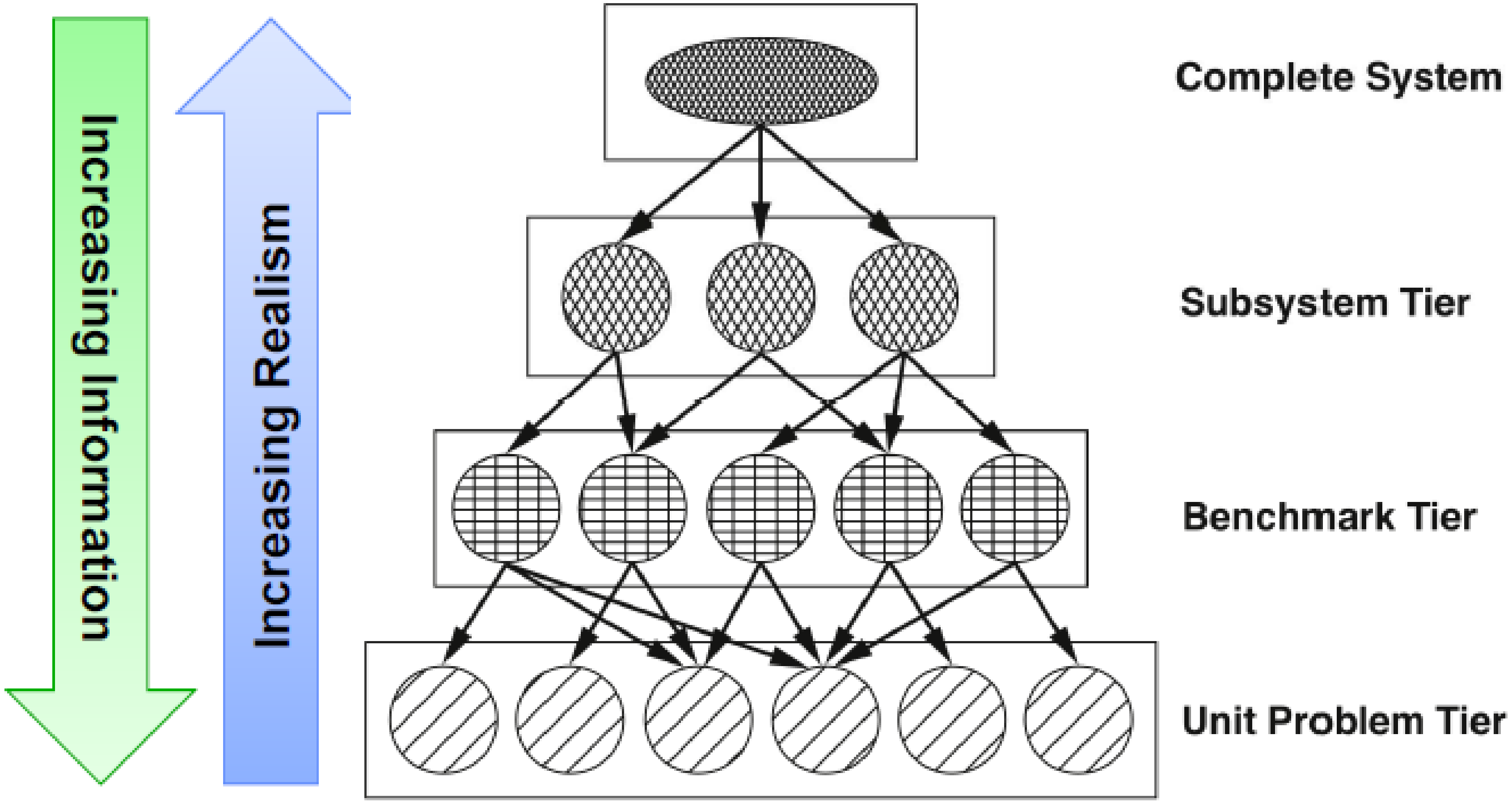
Experimental Activities:
- Experiment design
- Initial and boundary conditions
- Response measurements
- Uncertainty assessment

Validation

Application

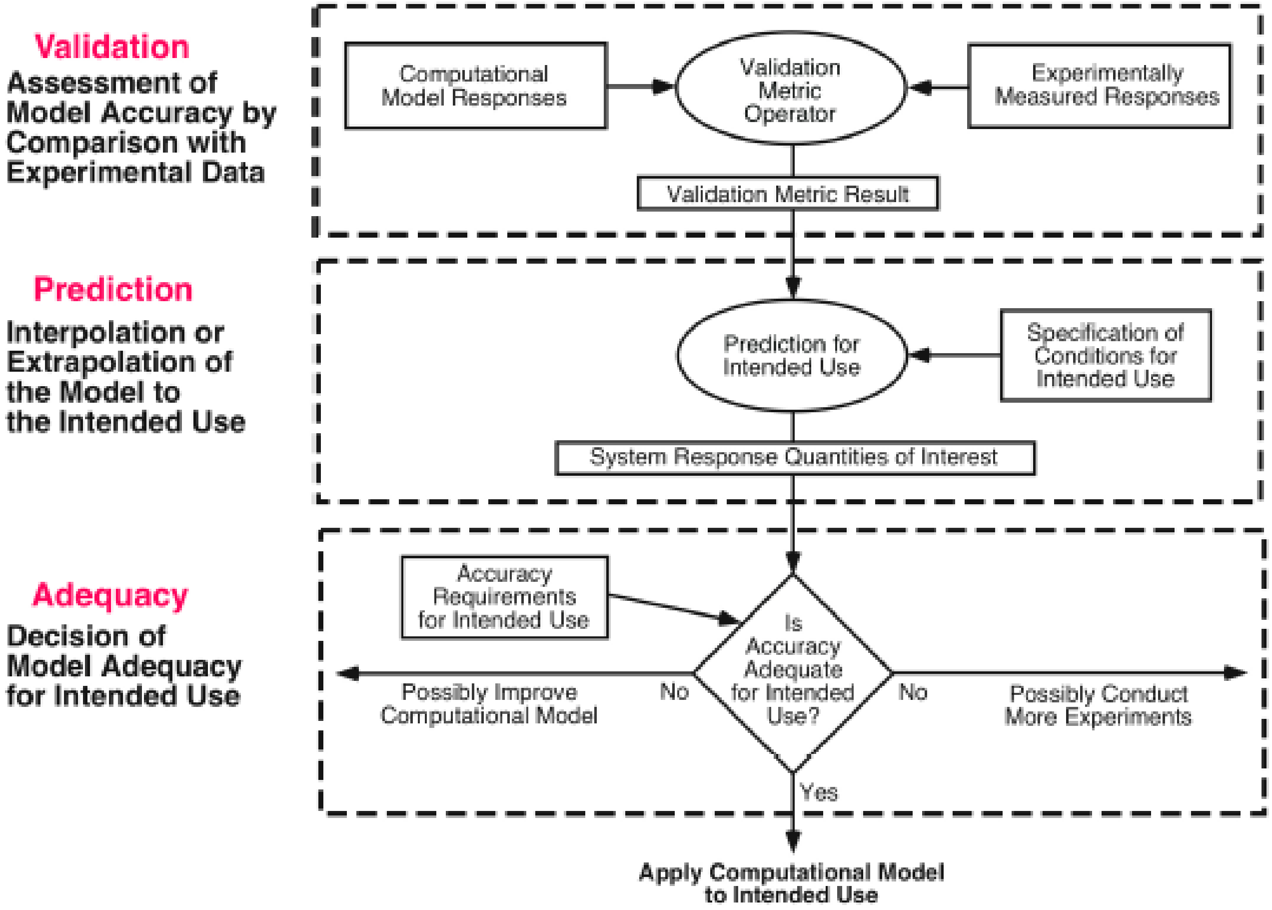
(Ref: ASME Guide, 2006)

Validation Hierarchy



(Ref: AIAA Guide, 1998)

Contrasting Validation, Prediction, and Model Adequacy



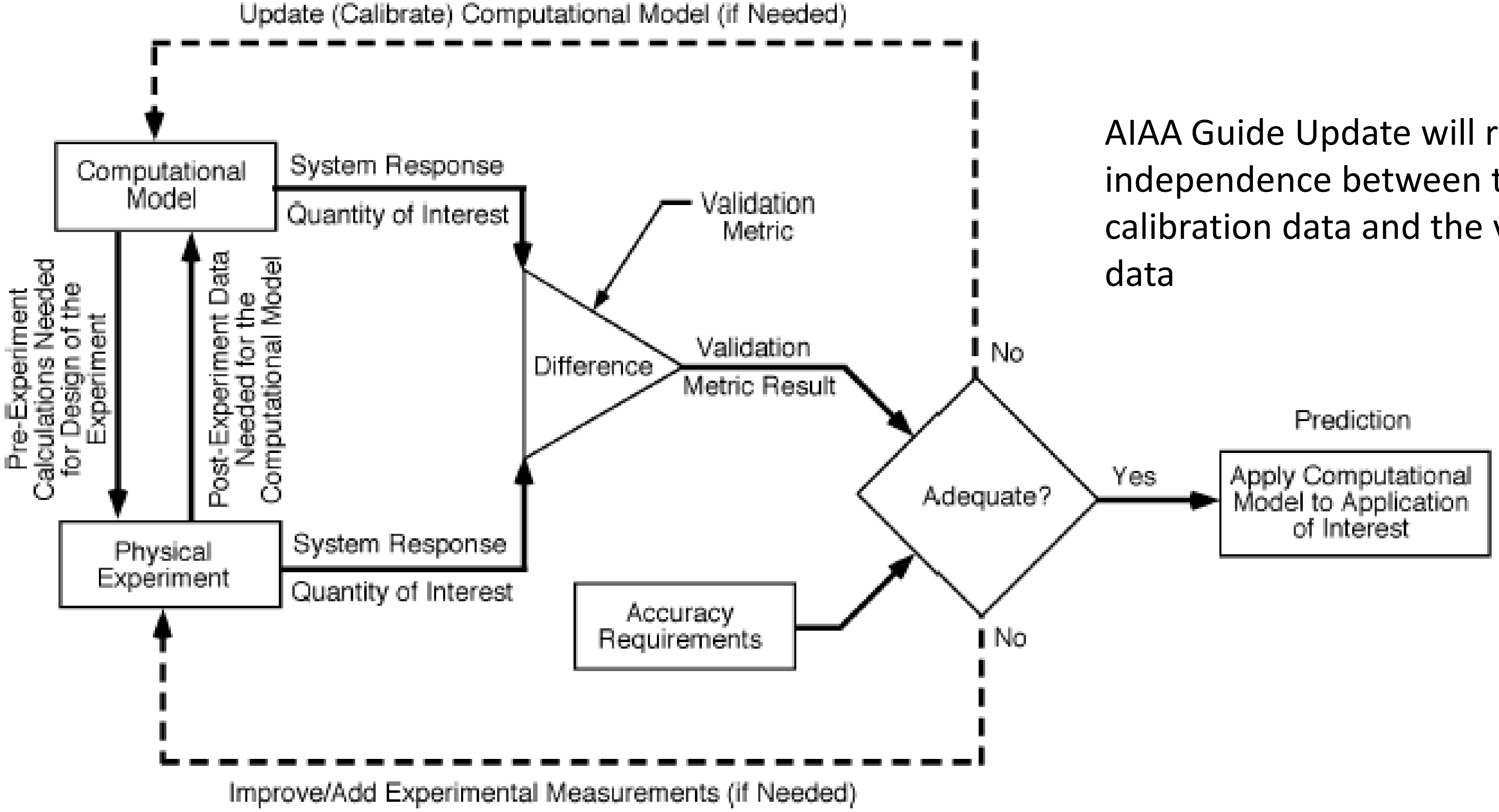
Model
Accuracy Assessment

Model
Prediction
(Extrapolation)

Model
Adequacy Assessment

(Ref: Oberkampf and Trucano, 2008)

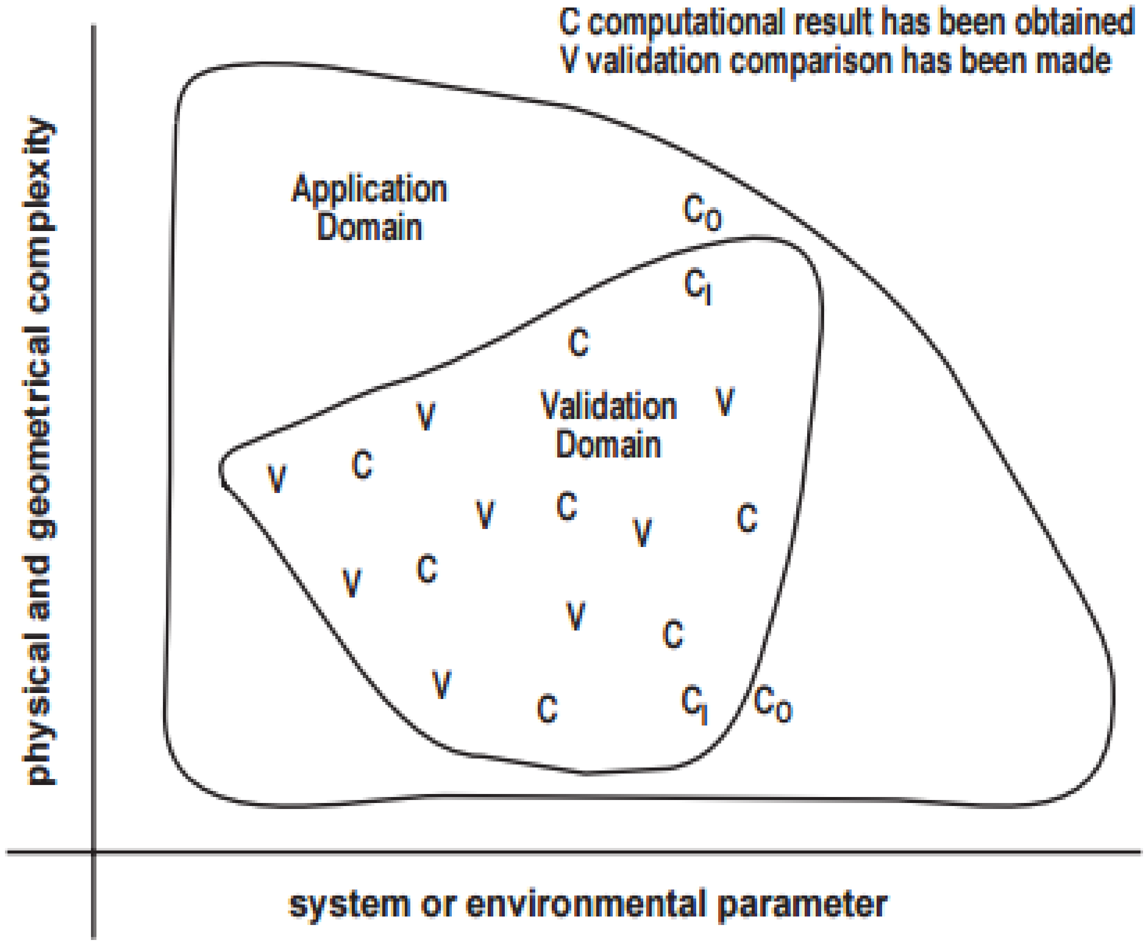
Model Accuracy Assessment, Calibration and Prediction



AIAA Guide Update will recommend independence between the calibration data and the validation data

(Ref: Oberkampf and Barone, 2006)

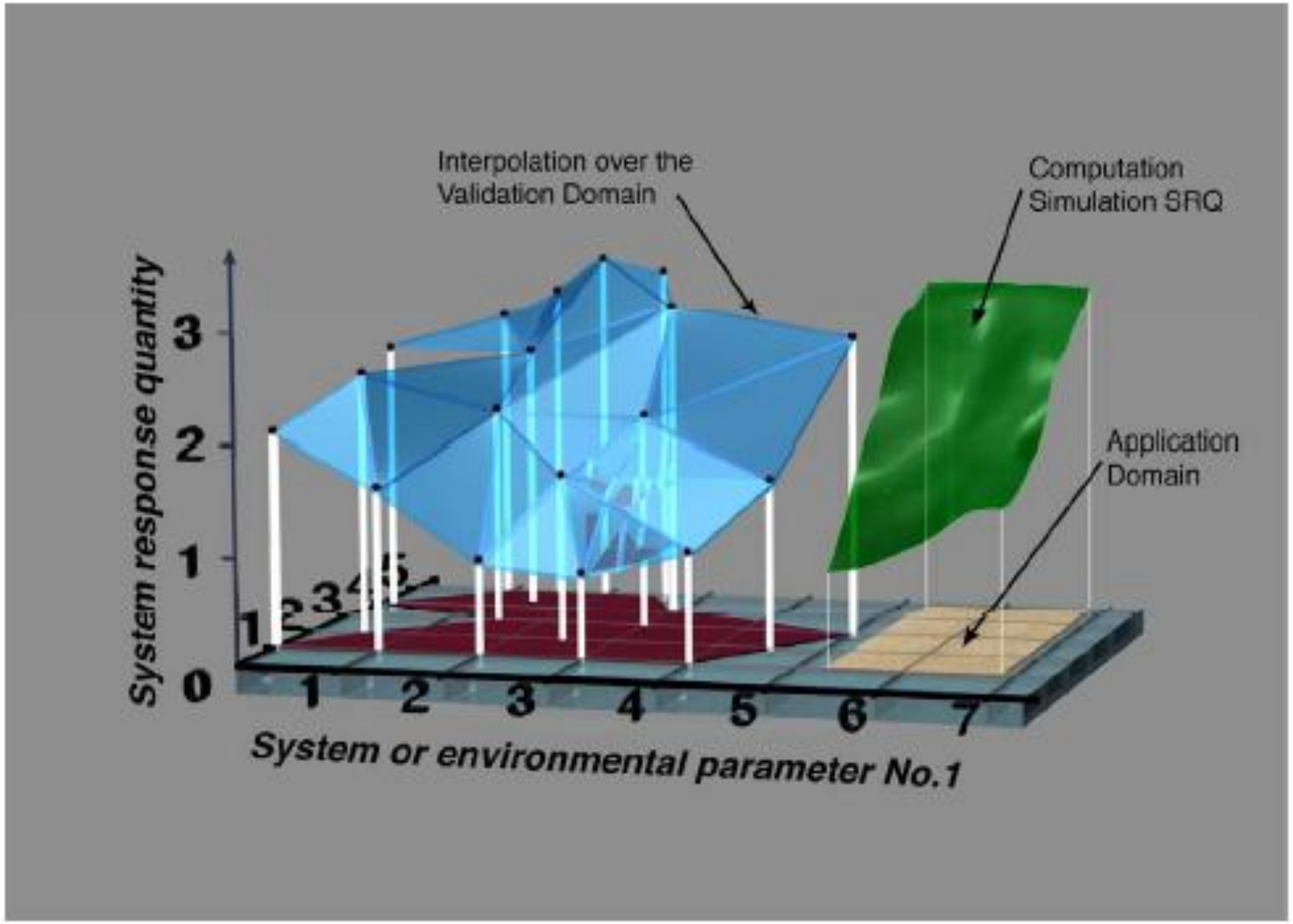
Model Accuracy Assessment Relative to Experimental Data



- Typical relationship between application domain and validation domain
- Typically application domain much larger than validation domain
- Model prediction:
  - Model extrapolation to intended application conditions (outside of the validation domain)

(Ref: Oberkampf, Trucano, and Hirsch, 2003)

Prediction Far From the Validation Domain: Extrapolation



(Ref: Oberkampf and Roy, 2010)

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

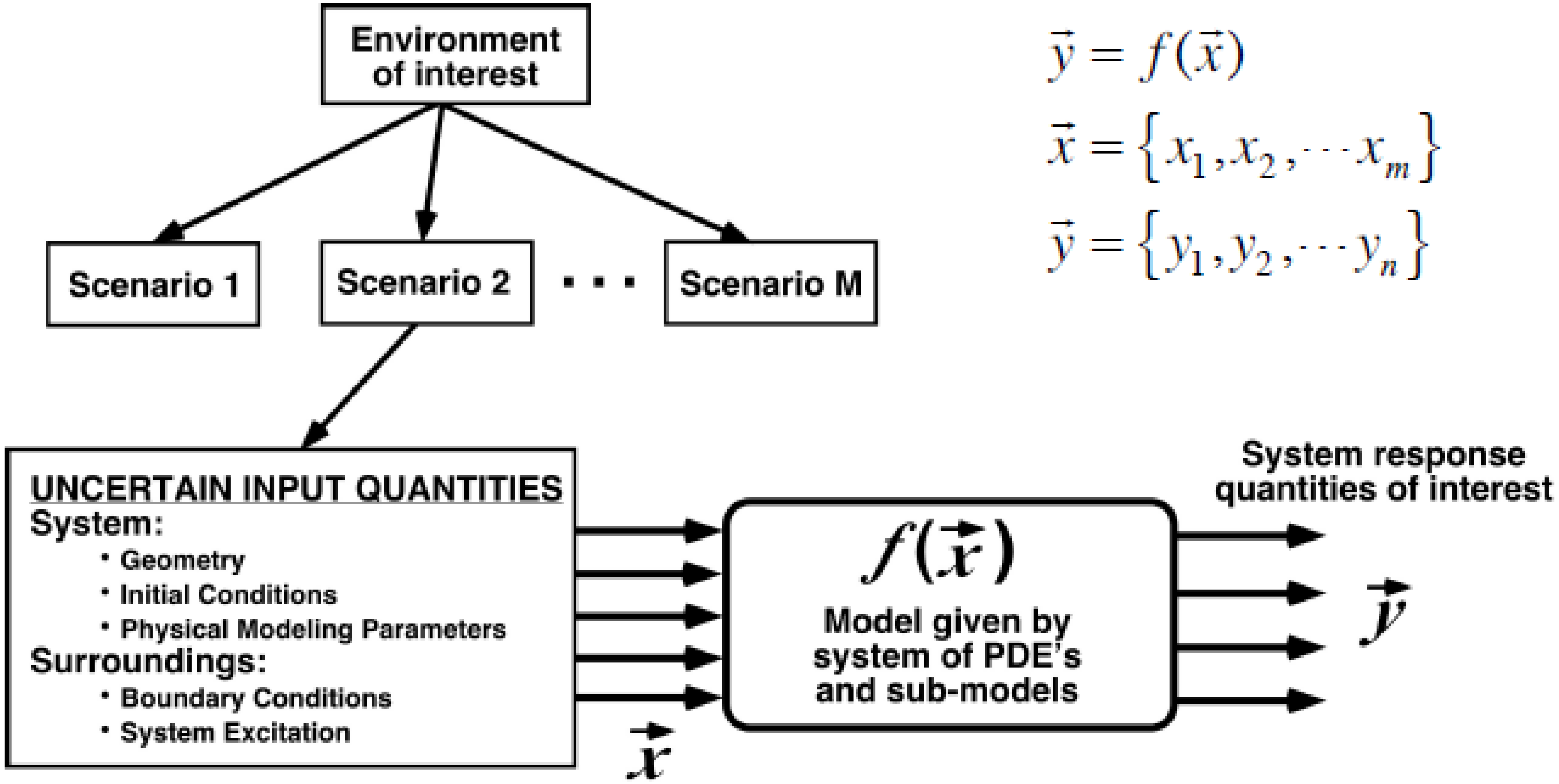
Predictive Capability and Uncertainty Quantification

Form of the equations:

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

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

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



Environment of interest

Scenario 1

Scenario 2

. . .

Scenario M

UNCERTAIN INPUT QUANTITIES

System:

- Geometry
- Initial Conditions
- Physical Modeling Parameters

Surroundings:

- Boundary Conditions
- System Excitation

$\vec{x}$

$f(\vec{x})$

Model given by system of PDE's and sub-models

System response quantities of interest

$\vec{y}$

(Ref: Oberkampf and Roy, 2010)

Sources of Uncertainty

- Uncertainty in input parameters (model and numerical):
    - Input parameters from the system and surroundings (independently measurable versus those that can only be determined by calibration using the model)
    - Uncertainty modeling parameters, e.g., mean and standard deviation
    - Numerical algorithm parameters, e.g., numerical damping parameter
- Numerical solution error:
    - Round-off error
    - Iterative error
    - Spatial, temporal, and energy partition discretization error
- Model form uncertainty:
    - Estimated at the conditions for validation experiments
    - Estimated or extrapolated to the application conditions of interest

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 in weather conditions, e.g., wind speed, rain fall, temperature
    - Variability in properties of natural and man-made materials
    - Variability in excitation, e.g., frequency and amplitude due to earthquakes
- **Epistemic uncertainty**: uncertainty due to lack of knowledge
  - Also referred to as reducible uncertainty, knowledge uncertainty, and subjective uncertainty

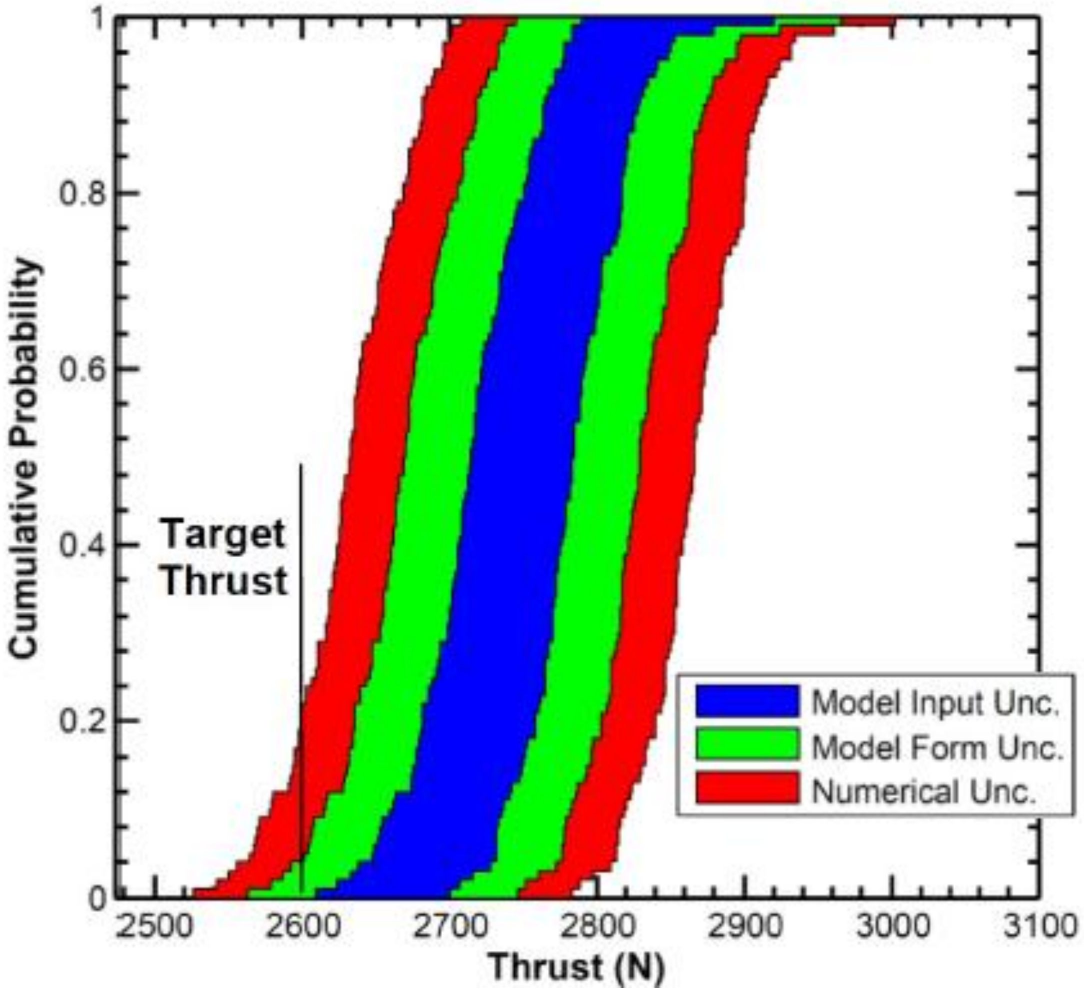
    Epistemic uncertainty is characteristic of our knowledge of the system
  - Examples:
    - Poor understanding of physical phenomena, e.g., fracture in composites
    - Poor understanding of accident scenarios and event/failure trees
    - Model form uncertainty, e.g., two-phase flow model closures

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

Approaches to Predictive Uncertainty

- Bayesian inference (after Kennedy and O’Hagan):
  - Every uncertainty is assumed to be random variable characterized as probability distribution
  - If little information is available for an uncertainty, a probability density function (PDF) is assumed
  - Emphasis is on:
    - Updating uncertain input parameters using available experimental data
    - Estimating model bias errors, i.e., model form uncertainty
- Imprecise probability theory:
  - Characterize epistemic uncertainty as an interval-valued quantity
  - Emphasis is on segregating aleatory and epistemic uncertainty
  - Evidence (Dempster-Shafer) theory and probability bounds analysis
- Use of competing models and model teams
  - Used in Waste Isolation Pilot Plant and Yucca Mountain performance assessments
  - Weather and hurricane tracking models

Example of a p-Box with Various Sources of Uncertainty



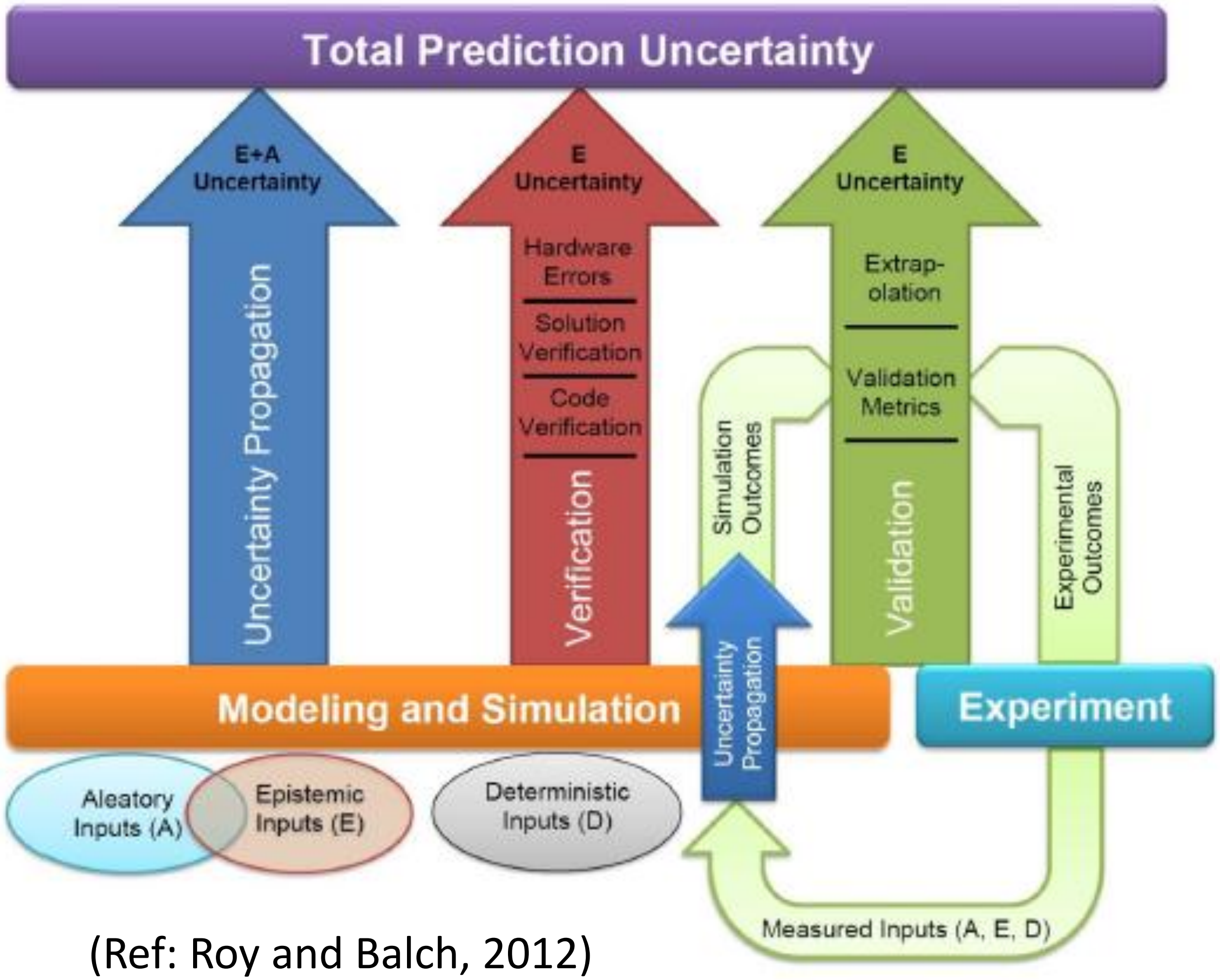
(Ref: Roy and Balch, 2012)

- Prediction of thrust from a small rocket motor
- Uncertain inputs to the mathematical model:
  - Total pressure in the motor
  - Expansion ratio of the nozzle
- Epistemic uncertainties in the simulations are:
  - Model form uncertainty
  - Numerical solution error

Predictive CFD: Verification, Validation, and Uncertainty Quantification of CFD

Three components to uncertainty quantification (UQ) in CFD:

- Numerical errors/uncertainty (verification)
- Modeling errors/uncertainty (validation)
- Propagation of input uncertainty



(Ref: Roy and Balch, 2012)

Concluding Remarks

- Code and solution verification must be practiced and improved to ensure we are building on solid foundation for simulation
- Validation is focused on assessing the accuracy of mathematical model vis-a’-vis experimental measurements
  - Validation experiments are commonly expensive, and they are not easy to conduct (even by experienced experimentalists)
- Predictive capability
  - Is focused on what we have never seen before
  - When we make predictions far from our validation database, we should concentrate on capturing total uncertainty
  - We should more widely embrace non-deterministic simulations:
    - This will be computationally expensive
    - Nondeterministic simulations will be at the expense of more complex models of physics

None of this will be easily accepted (by analysts or decision makers), nor will it be inexpensive