Verification and Validation in Computational Simulation

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Motivation

- Computational simulations have become a key contributor to:
  - Design and virtual prototyping of engineered systems
  - Supplementing experiments and testing of systems
  - Certification of the performance, safety, and reliability of high-consequence systems
- Why is verification and validation (V&V) important?
  - V&V procedures are the primary means of assessing accuracy in computational simulations.
  - V&V procedures are the tools with which we build confidence and credibility in computational simulations.
- The DOE Accelerated Strategic Computing Initiative (ASCI) is heavily investing in the research and development of V&V methodology and tools.

Outline of the Presentation

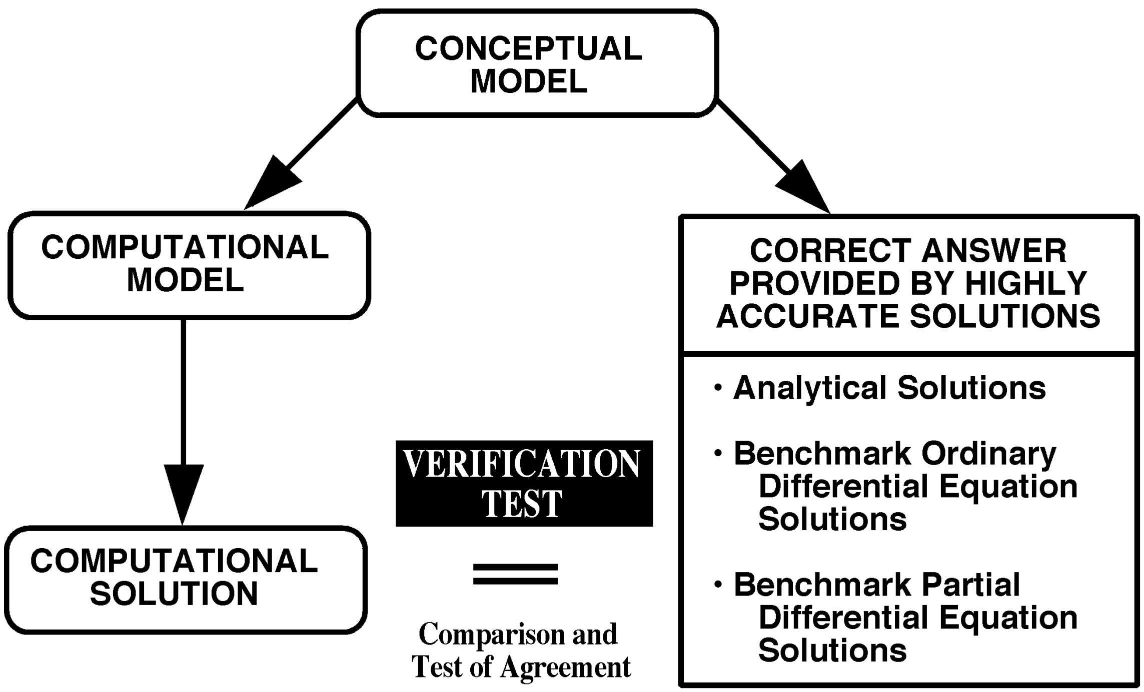
- **Terminology**
- **Code Verification**
- **Solution Verification**
- **Validation Fundamentals**
- **Validation Experiment Characteristics**
- **Closing Remarks**

Terminology: Verification

American Institute of Aeronautics and Astronautics, Committee on Standards in Computational Fluid Dynamics definition (1998):

Verification: **The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model**

Verification deals with mathematics



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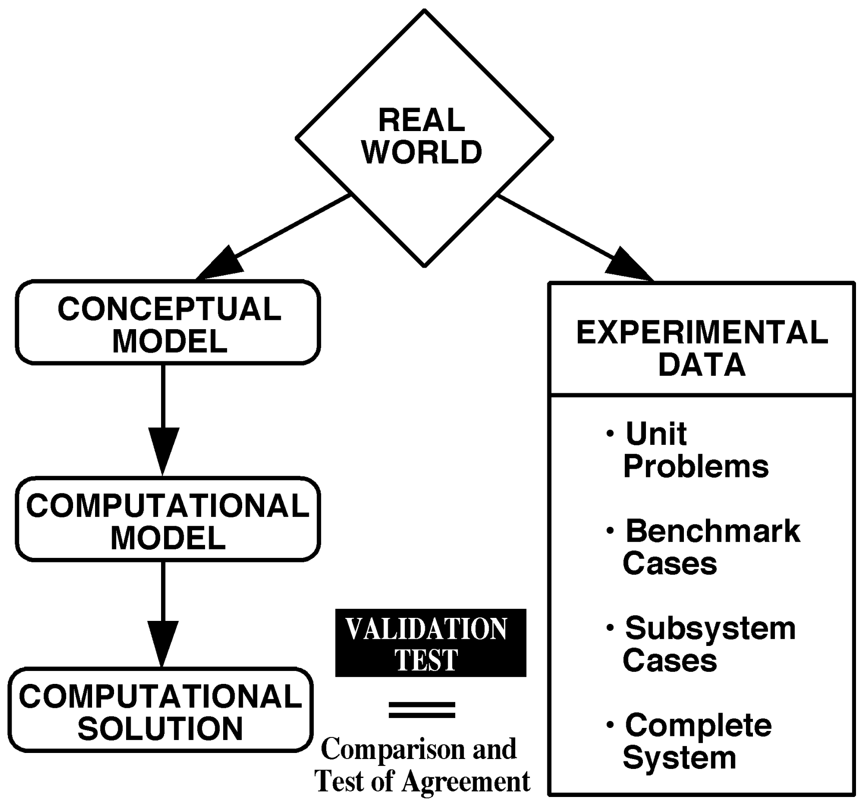
Two Types of Verification

- Verification is now commonly divided into two types:
- Code Verification: Verification activities directed toward:
  - Finding and removing mistakes in the source code
  - Finding and removing errors in numerical algorithms
  - Improving software using software quality assurance practices
- Solution Verification: Verification activities directed toward:
  - Assuring the accuracy of input data for the problem of interest
  - Estimating the numerical solution error
  - Assuring the accuracy of output data for the problem of interest

Definition of Validation

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



Important Features of Verification and Validation

- Both definitions stress "process of determining":
  - Each process provides evidence (substantiation)
  - The veracity, correctness, or accuracy of all possible solutions to the conceptual model cannot be proven
- Both definitions stress comparison with a reference standard:
  - A measurement of accuracy, or error, must be available
  - For verification, the standard is the "conceptual model"
  - For validation, the standard is the "real world"

Verification provides evidence that the computational model is solved correctly and accurately.

Validation provides evidence that the mathematical model accurately relates to experimental measurements.

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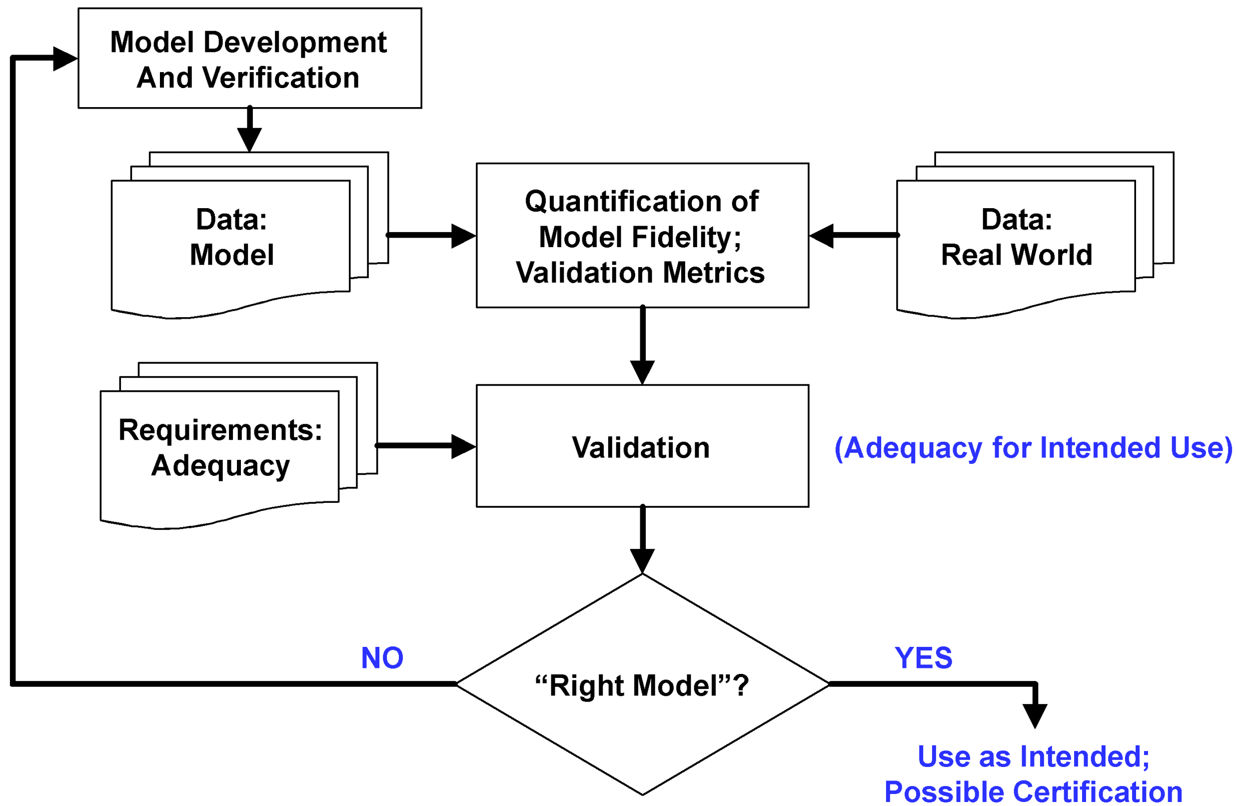
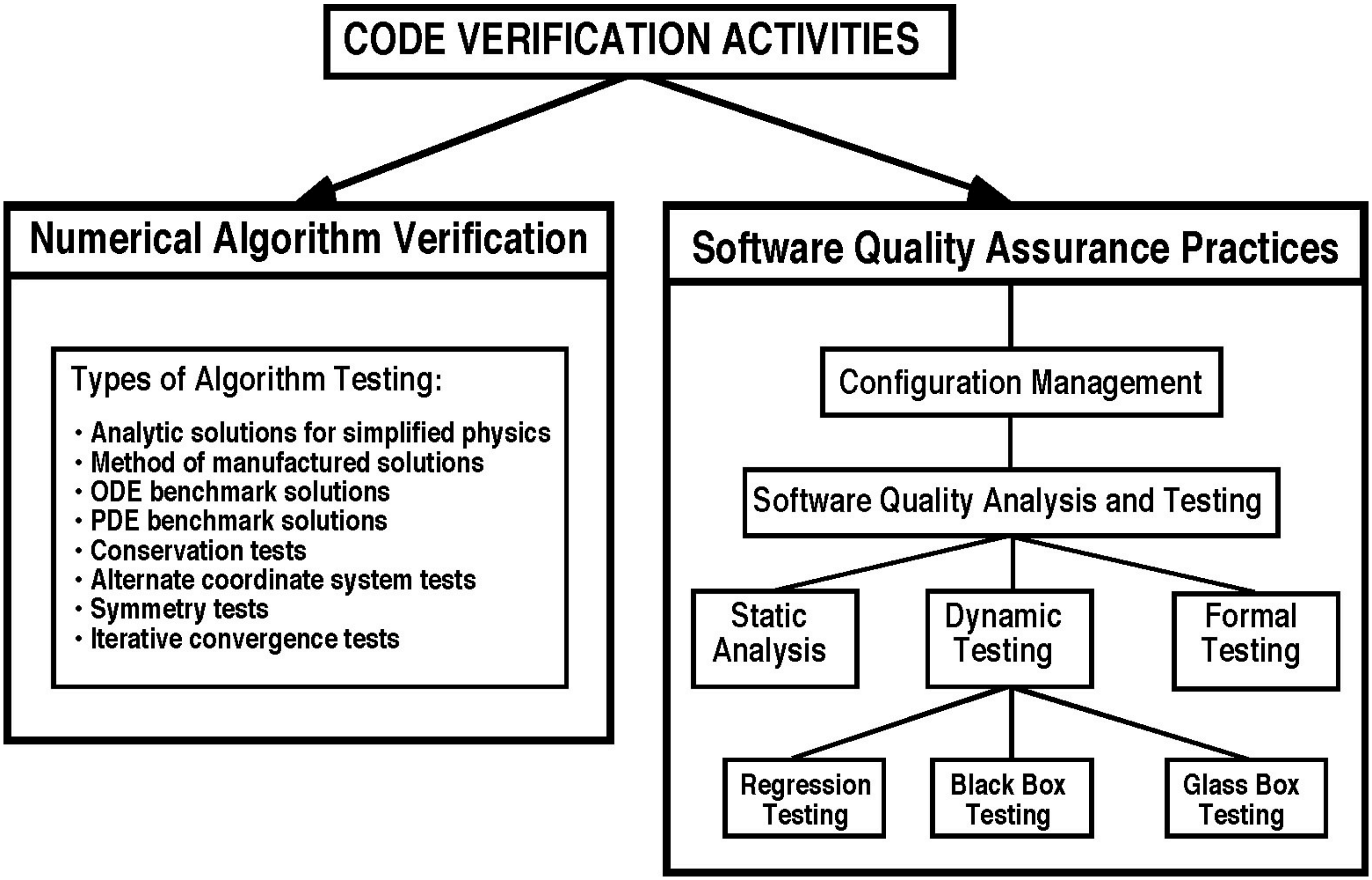
Model Fidelity and Model Validation (ASME Committee on V&V in CSM, 2003)



Code Verification



Numerical Algorithm Verification

- **Formal order of accuracy of a numerical method is determined by:**
  - **Taylor series analysis for finite-difference and finite volume methods**
  - **Interpolation theory for finite-element methods**
- **Consider the 1-D unsteady heat conduction equation:**

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0$$

- **Using a forward difference in time and a centered difference in space, the Taylor series analysis results in:**

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = \left[-\frac{1}{2} \frac{\partial^2 T}{\partial t^2} \right] \Delta t + \left[\frac{\alpha}{12} \frac{\partial^4 T}{\partial x^4} \right] (\Delta x)^2 + O\left(\Delta t^2\right) + O\left(\Delta x^4\right)$$

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Observed Order of Accuracy

- **Computed solutions do not typically reproduce the formal order of accuracy**
- **Factors that can degrade the formal order of accuracy include:**
  - **Mistakes in the computer code, i.e., programming errors**
  - **Δx, Δy, Δz, Δt are not sufficiently small for the solution to be in the asymptotic convergence region, i.e., truncation errors**
  - **Singularities or discontinuities in the solution domain and on the boundaries**
  - **Insufficient iterative convergence for solving nonlinear equations**
  - **Round-off error due to finite word length in the computer**
- **We use the term "observed" order of accuracy for the actual accuracy determined from computed solutions**

Methods for Determining the Observed Order of Accuracy

- **Method of Exact Solutions (MES):**
  - **MES involves the comparison of a numerical solution to the exact solution to the governing PDEs**
  - **MES is the traditional method for code verification testing**
  - **Number and variety of exact solutions is extremely small**
- **Method of Manufactured Solutions (MMS):**
  - **MMS is a more general and more powerful approach for code verification**
  - **Rather than trying to find an exact solution to a PDE, we "manufacture" an exact solution *a priori***
  - **It is not required that the manufactured solution be physically real**
  - **Use the PDE operator to analytically generate source terms in a new PDE**
  - **The manufactured solution is the exact solution to a new (modified) equation: original PDE + source terms**
  - **MMS involves solving the backward problem: given an original PDE and a chosen solution, find a modified PDE which that chosen solution will satisfy**
  - **Initial & boundary conditions are determined from the solution, after the fact**

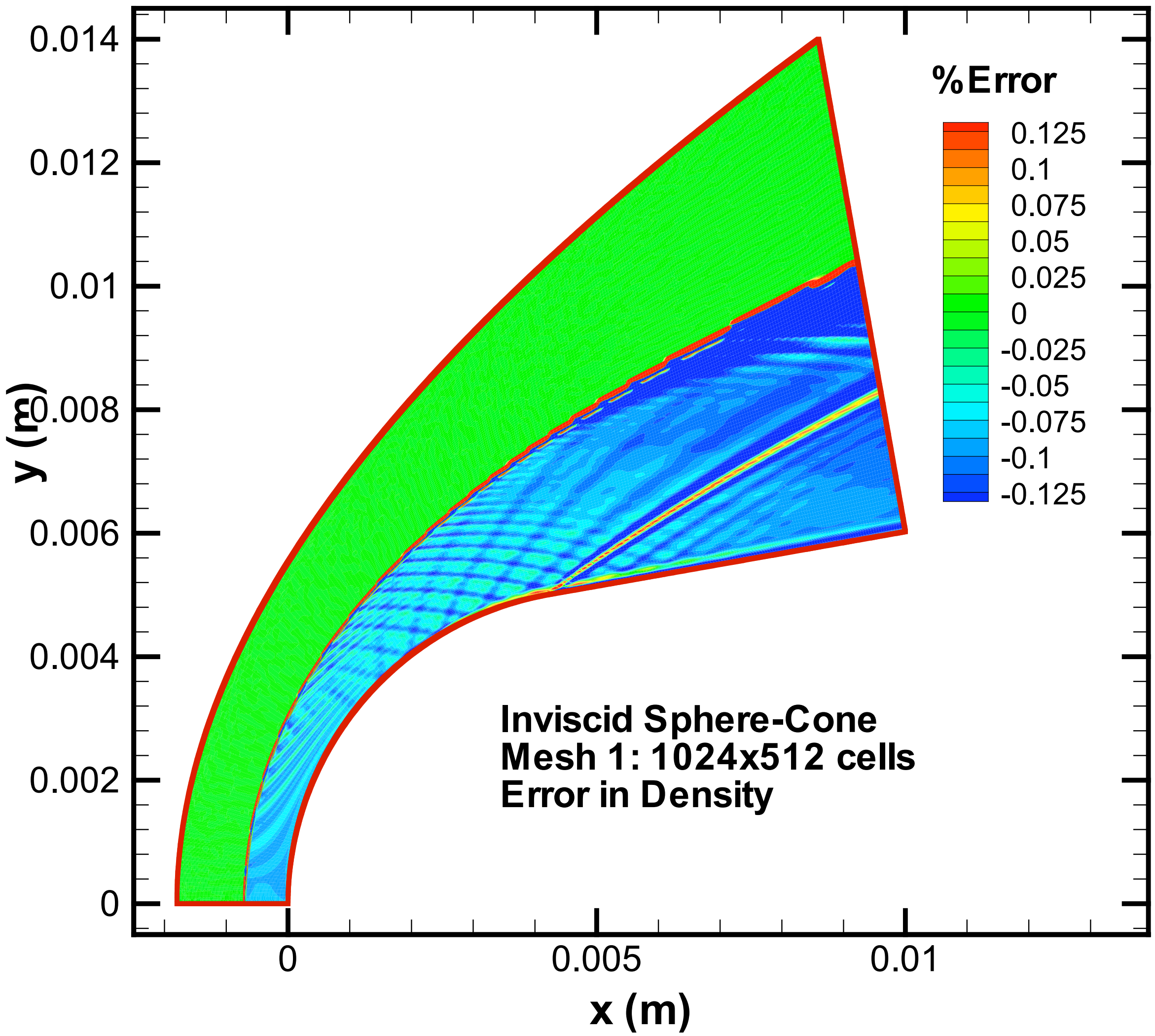
Solution Verification

- **Three aspects of solution verification:**
  1. **Verification of input data**
     - **Ensuring correct input files, grids, physical and material data, etc.**
  2. **Numerical error estimation of the solution**
     - **Mapping from continuum mathematics to discrete mathematics**
     - **Non-zero Δx, Δy, Δz, Δt**
     - **Insufficient iterative convergence for solving nonlinear equations**
     - **Round-off error due to finite word length in the computer**
  3. **Verification of output data**
     - **Ensuring that the correct files are used and post-processing steps taken**
- **Solution verification must be performed for every simulation that is sufficiently different from previous solutions**

Numerical Solution Error

- Discretization error (DE) arises due to the mapping of PDEs to discretized equations
- The DE can be clearly related to the truncation error (TE) using a Taylor series expansion for linear PDEs
- For nonlinear problems, the relation between DE and TE is not as straightforward (Celik and Hu, 2003)
- Discretization of the boundary conditions can dominate the numerical accuracy if the the order of accuracy is less than the interior scheme
- The total (or global) DE is made up of two components
  - Local DE due to the local element size
  - Error that has been transported from other regions (also known as pollution error)

Local and Transported Error (Roy, 2003)



- **Mach 8 flow over a spherically-blunted-cone**
- **Local DE sources:**
  - **Capturing of the bow shock wave**
  - **Sphere-cone tangency point**
- **Error is also transported**
  - **By convection along streamlines**
  - **Along Mach waves in supersonic flow**

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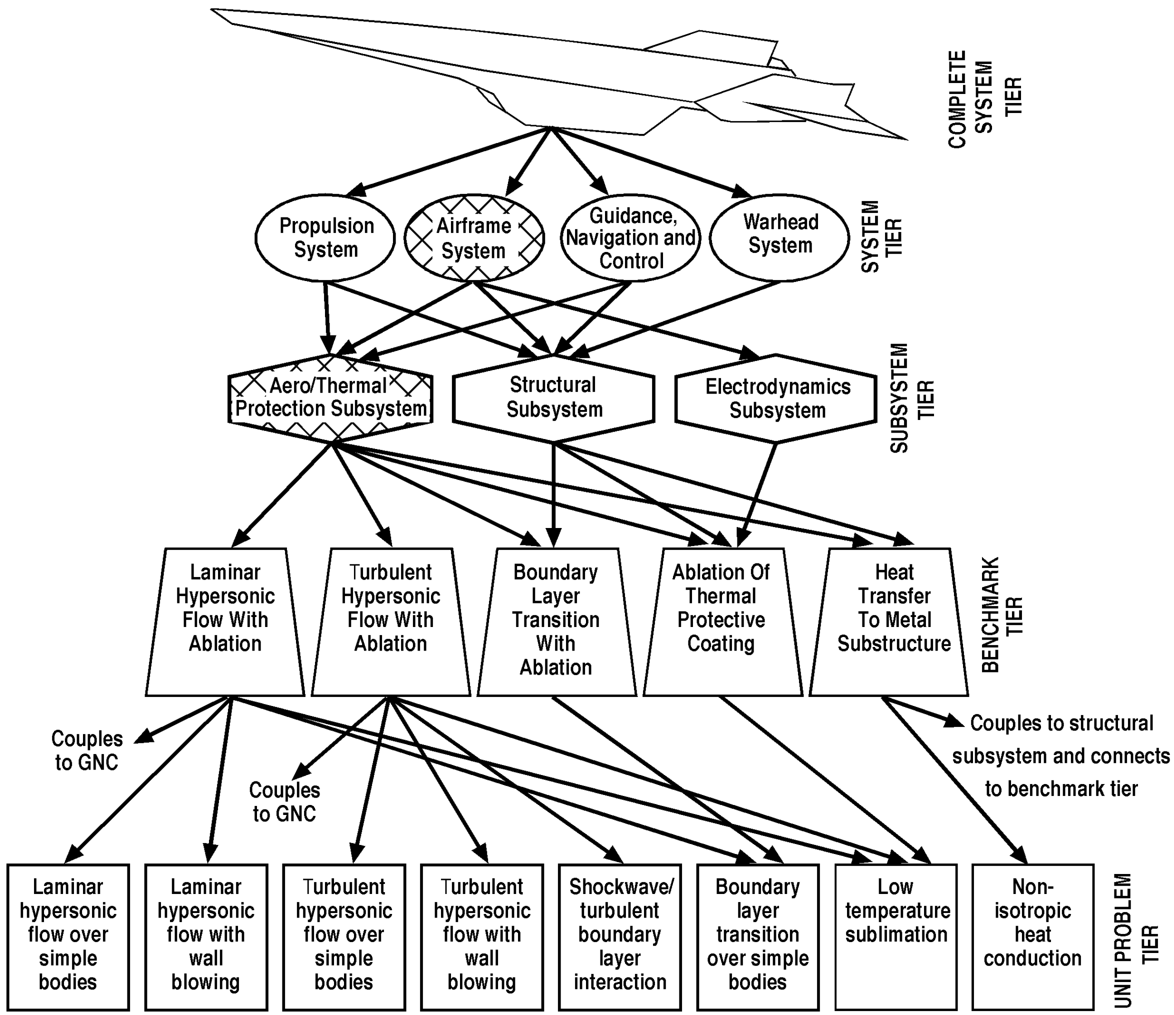
Approaches for Estimation of Discretization Error

- *a priori* error estimation:
  - Estimated before the numerical solution is computed
  - Estimated by truncation error analysis for finite difference or finite volume scheme
  - Estimated by interpolation theory for finite element schemes
  - Not useful for practical problems because the magnitude of the error is only know within a (unknown) constant
- *a posteriori* error estimation
  - Estimated after at least one numerical solution is computed
  - Finite-element-based error estimation
    - Recovery methods: e.g., Zienkiewicz-Zhu (1992)
    - Residual methods, adjoint methods
  - Extrapolation-based error estimation
    - Richardson extrapolation (h-extrapolation)
    - Order extrapolation (p-extrapolation)

Validation Fundamentals

- Goals of validation:
  - Tactical goal: Characterization and minimization of uncertainties and errors in the computational model as well as in the experimental data
  - Strategic goal: Increase confidence in the quantitative predictive capability of the computational model
- Validation procedure does not imply that the experimental data is always correct:
  - Experimental uncertainty estimates may be very large
  - Unknown bias errors can exist in the experimental data
- Validation experiments:
  - Can be conducted at different levels in a hierarchy of complexity
  - Various system response quantities can each be used in a validation metric

Validation Experiment Hierarchy



Traditional Experiments vs. Validation Experiments

Three types of traditional experiments:

1. **Improve the fundamental understanding of the physics:**
   - **Ex: Fluid dynamic turbulence experiment, experiment for understanding the decomposition of a thermal protection material**
2. **Improve the mathematical models of some physical phenomena:**
   - **Ex: Detonation chemistry experiment, multi-phase flow experiment**
3. **Assess subsystem or complete system performance:**
   - **Ex: Performance of the National Ignition Facility**

- **Model validation experiment**
  - **An experiment that is designed and executed to quantitatively estimate a mathematical model's ability to simulate a physical system or process.**
- **The computational model developer/code user is the customer.**

Why is it Difficult to Use Existing Experimental Data for Model Validation?

The most common reasons are (in priority order):

1. Incomplete measurement or documentation of model input quantities:
   - BCs and ICs (including actual geometry and facility imperfections)
   - Physical/material properties
   - System excitation or imposed electromagnetic fields
2. Limited measurement of system output quantities:
   - Typically only global or high-level quantities are measured
3. Limited experimental uncertainty estimates and documentation of:
   - Random error
   - Bias error (Ex: diagnostic technique, facility imperfections)
   - Unit-to-unit or setup-to-setup variability

Validation Experiment Characteristics

1. A validation experiment should be jointly designed and executed by experimentalists and computationalists:
   - Close working relationship from inception to documentation
   - Complete candor concerning strengths and weaknesses
2. A validation experiment should be designed to capture the relevant physics, all initial and boundary conditions, and auxiliary data:
   - All important modeling input data must be measured in the experiment and key modeling assumptions understood
   - Characteristics and imperfections of the experimental facility should be included in the model, if possible

Characteristics of a Validation Experiment (continued)

3. **A validation experiment should use any possible synergisms between experiment and computational approaches:**
   - Offset strengths and weaknesses of computation and experiment
   - Use high confidence simulations for simple physics to calibrate or improve the characterization of the facility
4. **Independence between computational and experimental results should be maintained where possible:**
   - The flavor of a blind comparison should be maintained, I.e., input data is provided but not measured system response quantities
   - The computational simulation should be a prediction, not a calibration of the physics or the numerics

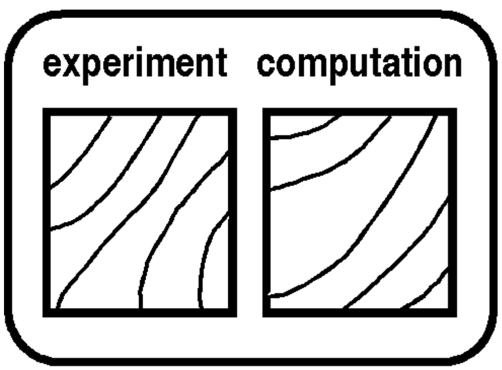
Characteristics of a Validation Experiment (continued)

5. A hierarchy of experimental measurements should be made which presents an increasing range of computational difficulty:
   – Functionals, local variables, derivatives of local variables.
   – Computational solution data should be processed in a manner similar to the experimental measurement data
6. Develop and employ experimental uncertainty analysis procedures to estimate random and correlated bias errors:
   – Use traditional, i.e., error propagation, or modern statistical methods to estimate random and correlated bias errors in both input and system response measurements
   – If possible, conduct experiments using different diagnostic techniques or in different experimental facilities

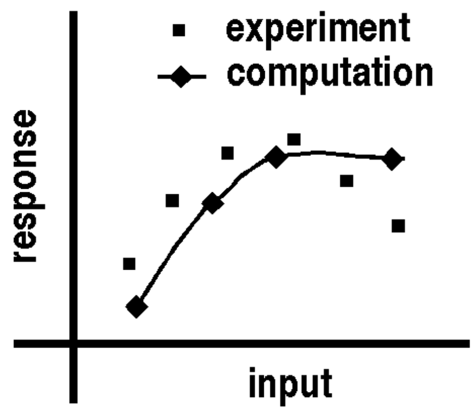
Traditional Methods for Comparing Computational Simulations and Experiments

Traditional methods of measuring the accuracy of computational results have been either qualitative or semi-quantitative

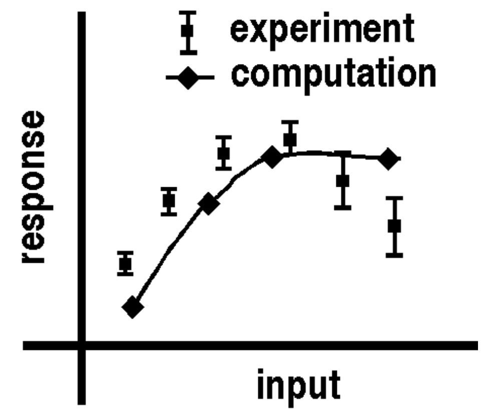
Some examples are:



(a) Viewgraph Norm



(b) Deterministic

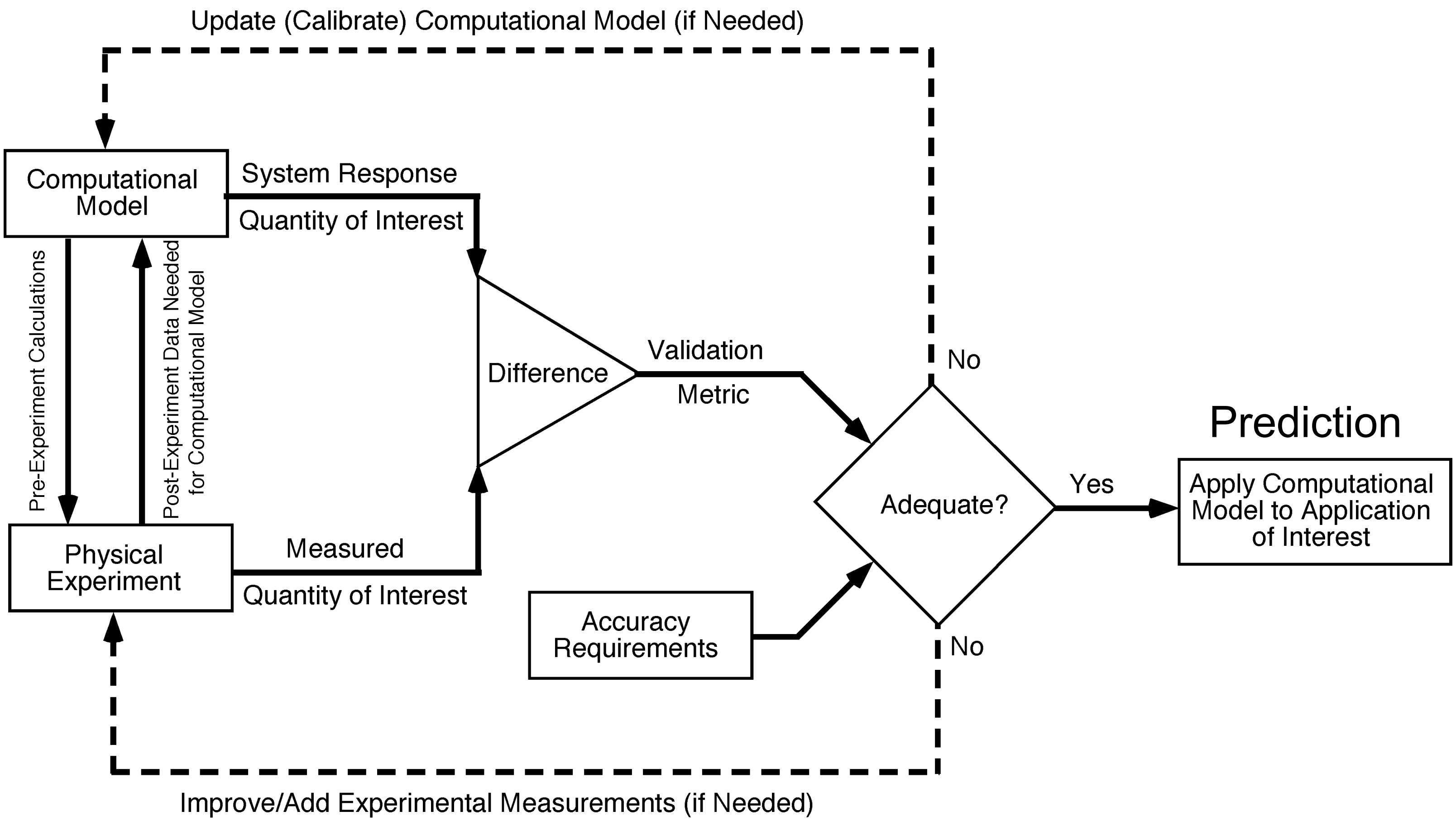


(c) Experimental Uncertainty

Validation Metrics are Quantitative Measures

- Validation metrics are measures of agreement between computational results and experimental measurements for system response quantities of interest
- Steps required to evaluate a validation metric:
  1. Choose a system response quantity (or multiple quantities) of interest
  2. Experimentally measure all input quantities needed for the code
  3. Experimentally measure the system response and estimate uncertainties
  4. Using the code and the input quantities from the experiment, compute the system response quantity
  5. A difference is computed between the experimental measurements, typically the estimated mean of the system response, and the computational results
- Validation metrics have been formulated using:
  - Bayesian updating (Hanson, Hasselman, Mahadevan)
  - Hypothesis testing (Hills and Trucano, Paez, Urbina, Rutherford, Dowding)
  - Statistical confidence interval methods (Easterling, Coleman, Oberkampf)

Relationship Between Validation, Calibration and Prediction



Closing Remarks

- Code verification is commonly assumed to have been completed by code developers:
  - This assumption is a serious mistake
  - Documented evidence should be required by code users
- Solution verification is commonly ignored by code users and decision makers:
  - This is a serious mistake
  - Evidence of solution verification should be required by decision makers
- Validation experiments are commonly expensive, and are they not easy to conduct (even by experienced experimentalists)
- Computational simulation should more widely embrace nondeterministic simulations:
  - This will be computationally expensive because of the additional numerical solutions required
  - Decision makers should require nondeterministic simulations to quantify uncertainties and system robustness
- None of this will be easily accepted

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Calibration

- For some cases when validation is not feasible or practical, calibration is appropriate
- AIAA Guide defined:

Calibration: The process of adjusting numerical or physical modeling parameters in the computational model for the purpose of improving agreement with real-world data

- Also known as: parameter estimation, model tuning, model updating

Calibration is a response to the "degree of representation of the real world" directed toward improvement of agreement.

- In many fields, calibration is critically important:
  - Calibration is commonly conducted before validation activities
  - Ex: In structural dynamics, determination of stiffness and damping in fastener joints and welds

Meaning of Prediction vs. Validation

Prediction refers to a simulation result for a specific case of interest that is different from cases that have been validated.

- Computationally replicating a point in the validation database is not a prediction

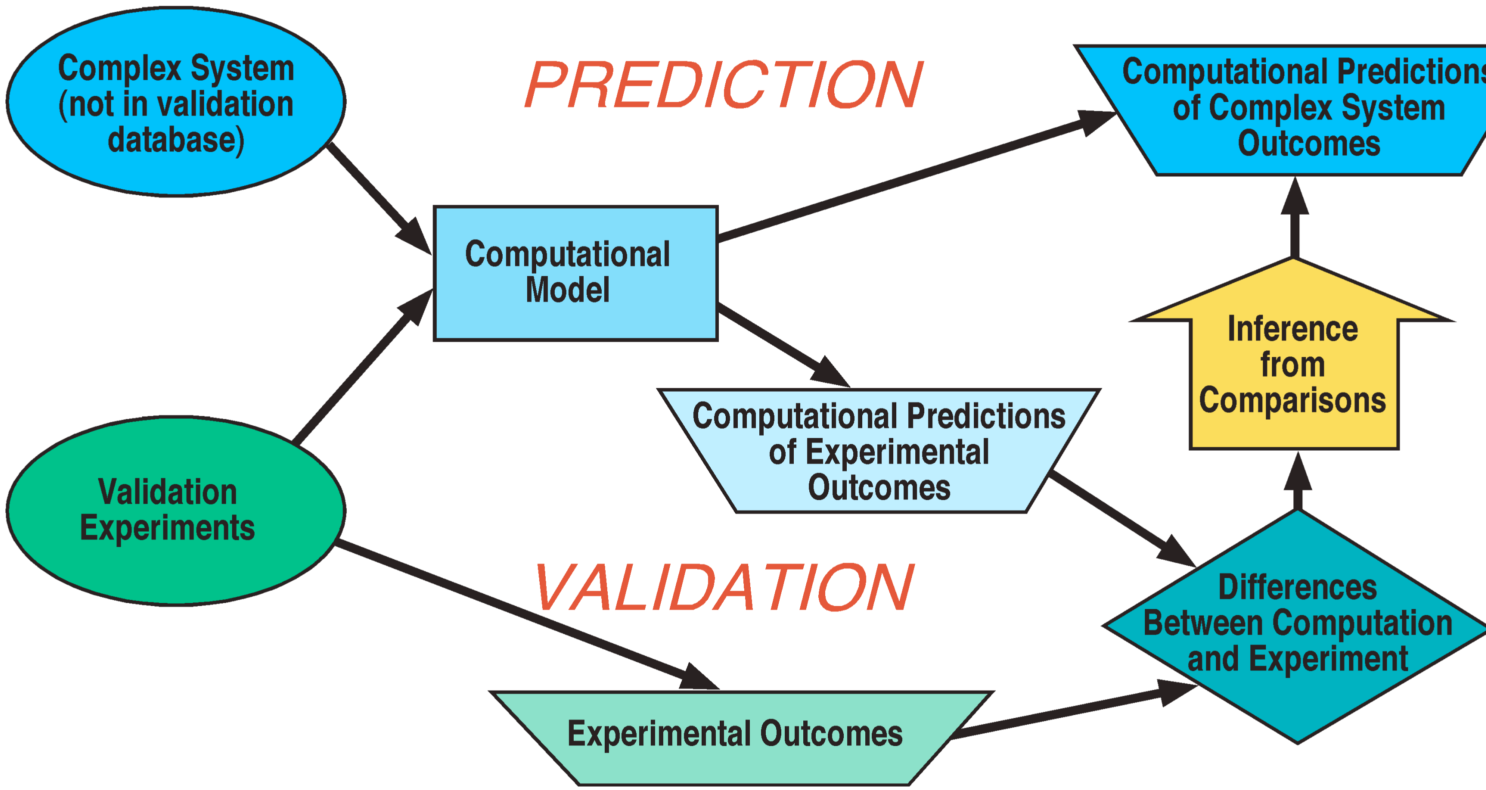
Validation should be viewed as a historical statement:

Reproducible evidence of measurable agreement between computational and experimental results

Validation does not directly make a claim about the accuracy of a prediction:

- Computational models are extremely general and easily misused (unintentionally and intentionally)
- How closely related are the conditions of the prediction and specific cases in the validation database?
- How well are the physics/chemistry of the process understood?

Relationship Between Validation and Prediction



Types of Error

Error: A recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge.

- Acknowledged errors are errors that can be estimated, bounded, or ordered
- Unacknowledged errors are mistakes or blunders

Examples of acknowledged errors:

- Finite precision arithmetic in a digital computer
- Insufficient spatial discretization
- Insufficient iterative convergence

Examples of unacknowledged errors:

- Computer programming errors (source code or compiler)
- Use of incorrect input files (geometry, material properties)

Types of Uncertainty

Aleatory uncertainty is the inherent variation associated with the physical system or the environment.

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

- **Examples:**
  - **Variation in thermodynamic properties due to manufacturing**
  - **Variation in joint stiffness and damping in structures**
  - **Random vibrational input to a structure**

Epistemic uncertainty is a potential deficiency in any phase of the modeling process that is due to lack of knowledge.

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

- **Examples:**
  - **Poor understanding of fracture dynamics**
  - **Poor knowledge or experience of failure, misuse, or hostile scenarios**
  - **Information obtained from expert-opinion elicitation**

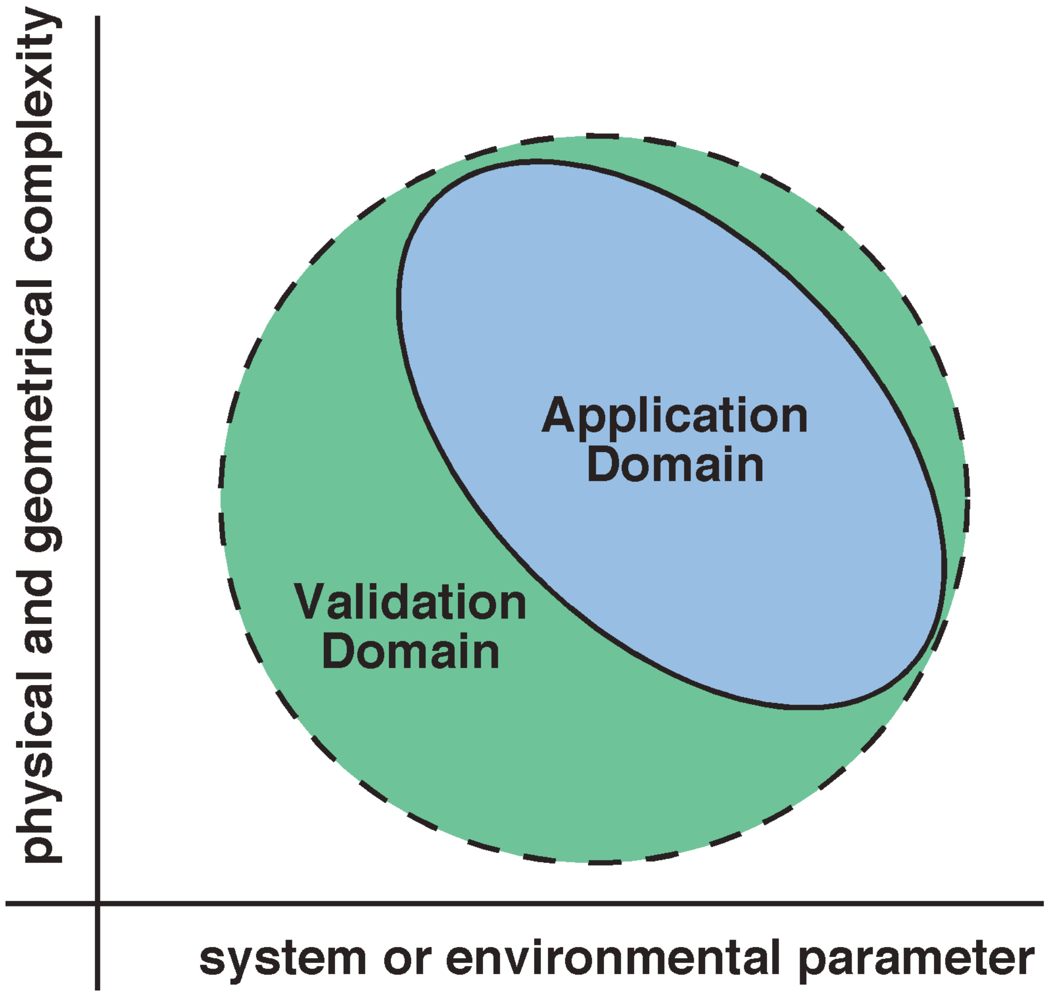
Software Quality Assurance (SQA)

- Formal procedures to ensure software is reliable
- Primarily developed by computer science community
- Driven by high consequence software systems
  - Aircraft automatic control systems
  - Autonomous vehicle control, such as spacecraft
  - Nuclear power plant control systems
- Configuration management
  - Concurrent Versions System (CVS) for software version control
  - Code documentation (requirements, equations, options)
- Software testing
  - Static testing
  - Dynamic testing
  - Formal testing

Recommended Characteristics for Validation Metrics

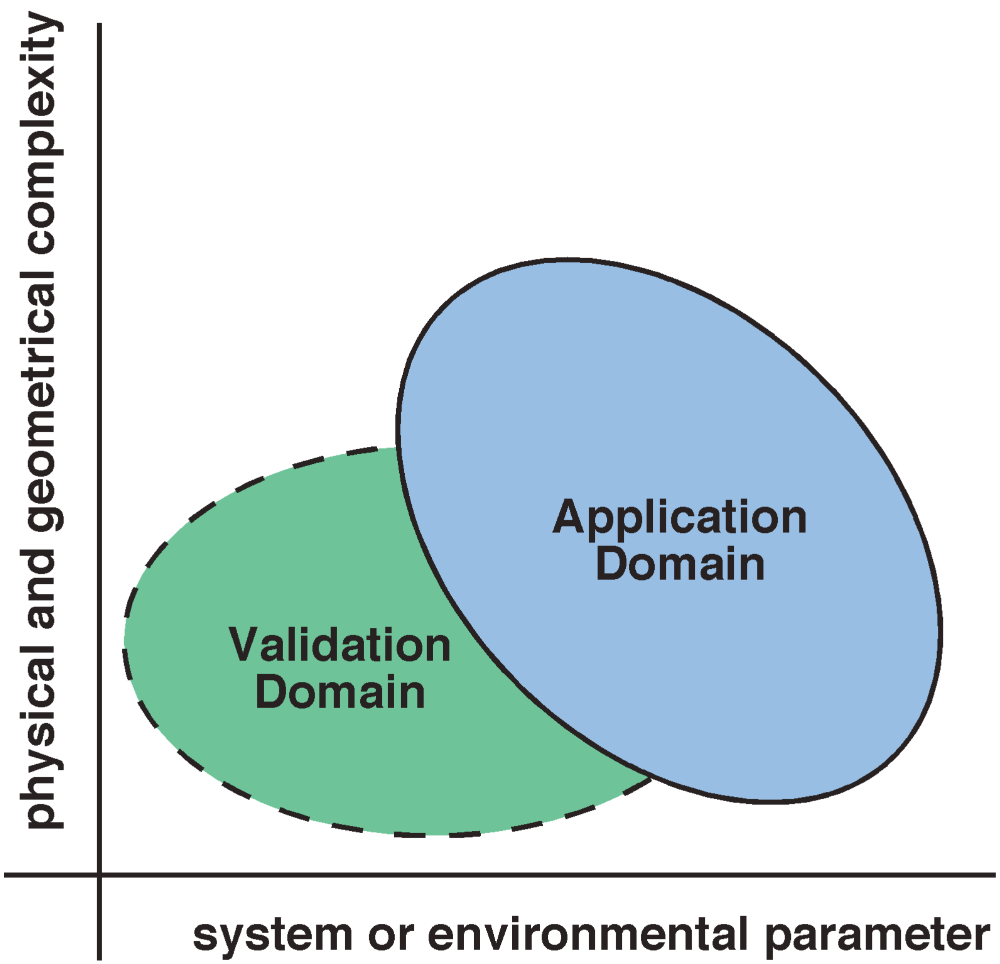
1) Should include an estimate of the numerical error (or show it is small) √
2) Should include an estimate of the experimental random errors and, if possible, the correlated bias errors √
3) Should include an accuracy assessment of the computational model, including all assumptions √
4) Should exclude a measure of adequacy of agreement between computational and experimental results √
5) Should depend on the number of experimental replications of a given experimental quantity √
6) Should depend on the uncertainty due to lack of experimental measurement of needed computational quantities and random uncertainty in experimental parameters

Traditional Engineering Inference: Interpolation



- **Complete overlap of application domain and validation database**
- **Prediction can be thought of as interpolation between points in the validation database**
- **Errors in the model are either:**
  - **Ignored (and the factor of safety in the design is increased)**
  - **Model is corrected using the bias error determined from the experiment**

Well-Founded Inference: Small Extrapolation



- Partial overlap of application domain and validation database
- Extrapolations typically occur in terms of various types of coordinate directions:
  - Input data for system parameters
  - Environmental parameters
  - Boundary conditions

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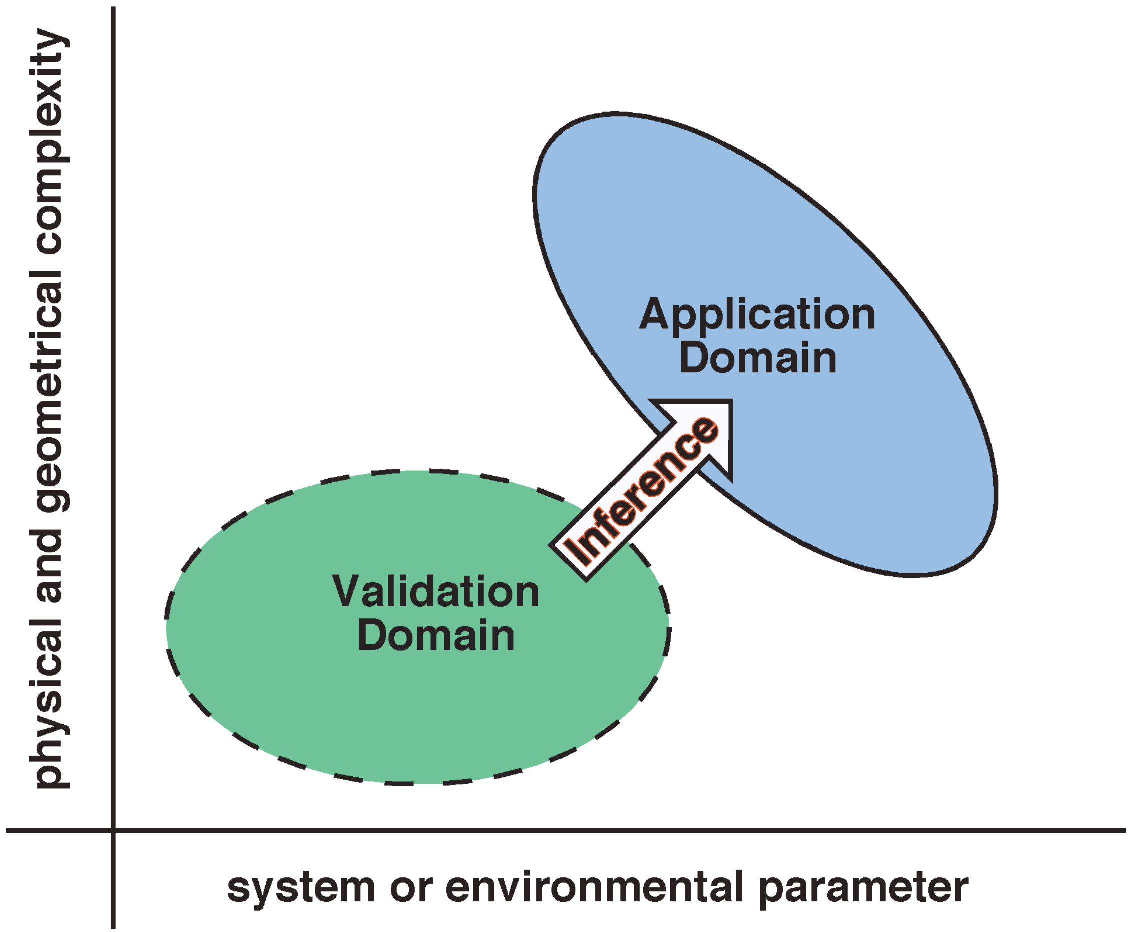
Weak Inference: Large Extrapolation



- No overlap of application domain and validation database
- Large extrapolations typically occur in terms of meta-coordinate directions, such as:
  - Large changes in physical complexity
  - Introduction of new physics coupling
  - Introduction of coupling between subsystems or components