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Perspective of Predictive Science in the NNSA Advanced Simulation and Computing Program

Dr. William L. Oberkampf

Distinguished Member Technical Staff
wloberk@sandia.gov

Dr. Anthony A. Giunta

Manager
Validation and Uncertainty Quantification Department
Sandia National Laboratories, Albuquerque, New Mexico
aagiunt@sandia.gov

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Outline of the Presentation

- **Background and Motivation**
- **Terminology and Methodology**
- **Elements of Predictive Capability**
- **Uncertainty Quantification**
- **Closing Remarks**

Background

- By Presidential decree, underground testing of nuclear weapons ceased in 1992.
- DOE/Stockpile Stewardship Program began in 1993 to insure the safety, reliability and performance of the nuclear stockpile
- The Accelerated Strategic Computing Initiative (ASCI) was initiated in 1996 (now called Advanced Simulation and Computing, ASC)
- Nuclear weapons labs: Sandia National Laboratories, Los Alamos National Laboratory, and Lawrence Livermore National Laboratory
- ASC Program components:
  - Defense Applications and Modeling
  - Integrated Computing Systems
  - Simulation and Computer Science
  - University Partnerships
- Roughly $7B has been spent as part of ASC program between the three weapons labs

ASC Program Elements

- **Defense Applications and Modeling elements:**
  - Materials and physics modeling
  - Physics-based applications software
  - Simulations of weapons systems, subsystems, and components
  - Verification and validation
- **Integrated Computing Systems**
  - Massively-parallel, computing platforms
- **Simulation and Computer Science**
  - Computer network systems
  - Visualization hardware and software
- **University Partnerships**
  - California Institute of Technology, University of Chicago, University of Illinois, Stanford University, and University of Utah
  - Proposals from roughly 20 universities are being reviewed for new awards

Motivation: Ensuring the Integrity of the Nuclear Stockpile

- **How can the safety, reliability, and performance (SRP) of the nuclear stockpile be assured without full system testing:**
  - **Inspection, monitoring and maintenance of weapons in the stockpile**
  - **Improved physics-based simulations to predict SRP**
  - **Comparison of simulations with:**
    - **Existing underground test database**
    - **New allowed testing of subsystems and components**
  - **Incorporation of V&V practices into decision making**
  - **Improved quantification of system margins and uncertainties (QMU)**
- **ASC approach to V&V:**
  - **Build on foundations of:**
    - **DOD/DMSO developed procedures**
    - **Techniques developed in computational fluid dynamics**
    - **Techniques developed for nuclear power reactor safety**
    - **Techniques developed for underground storage of nuclear waste**
  - **Develop improved V&V methodologies and procedures**
  - **Stronger emphasis on uncertainty quantification techniques**

Terminology: Verification

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.**

- **In computational science and engineering (CSE), two aspects of verification are recognized:**
- **Code Verification: Verification activities directed toward:**
  - **Finding and removing mistakes in the source code**
  - **Finding and removing errors in numerical solution algorithms**
  - **Improving software reliability using software quality engineering practices**
- **Solution Verification: Verification activities directed toward:**
  - **Assuring the accuracy of input and output data for the problem of interest**
  - **Estimating and reducing the numerical solution error, e.g. error due to finite element mesh resolution**

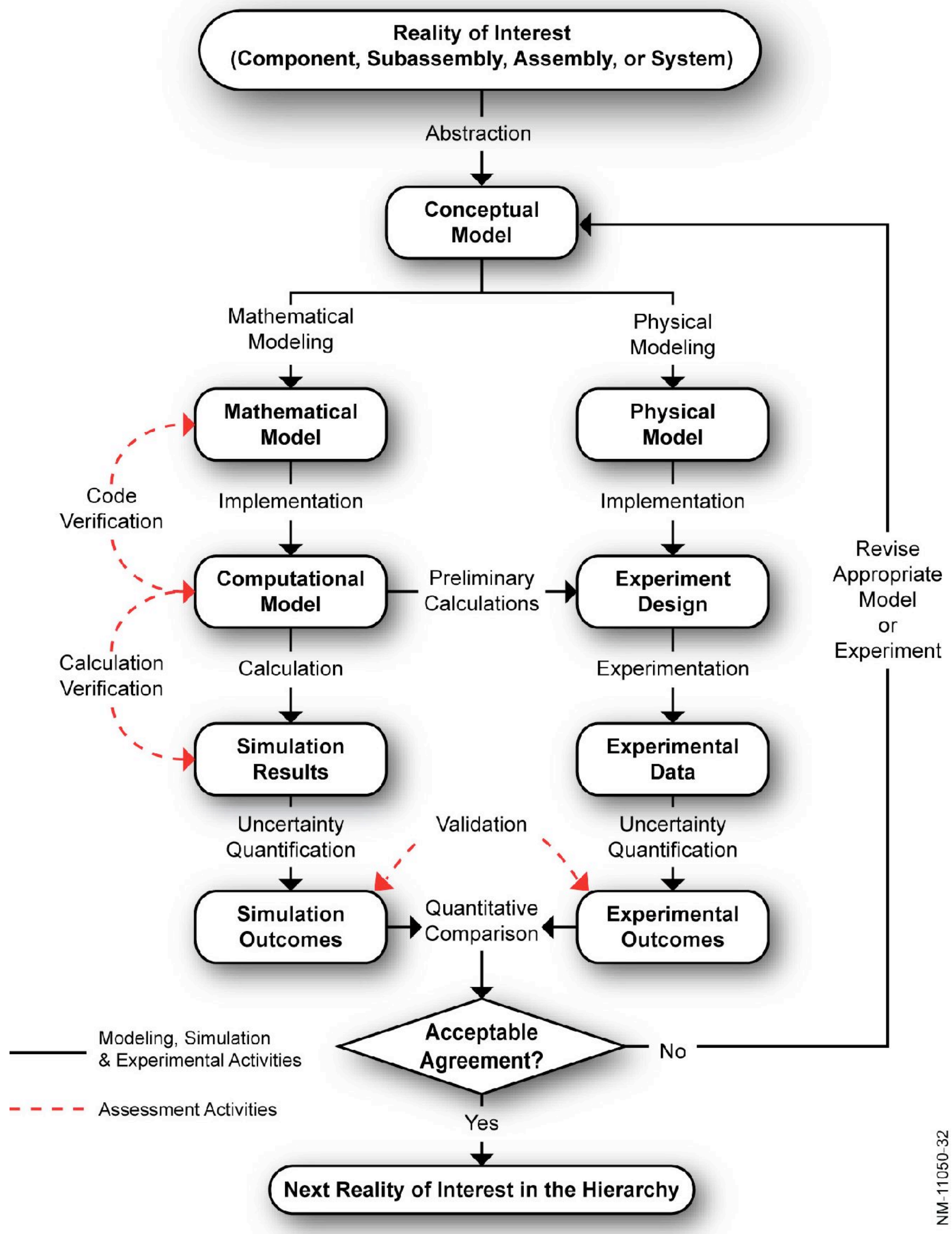
Terminology: Validation

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.

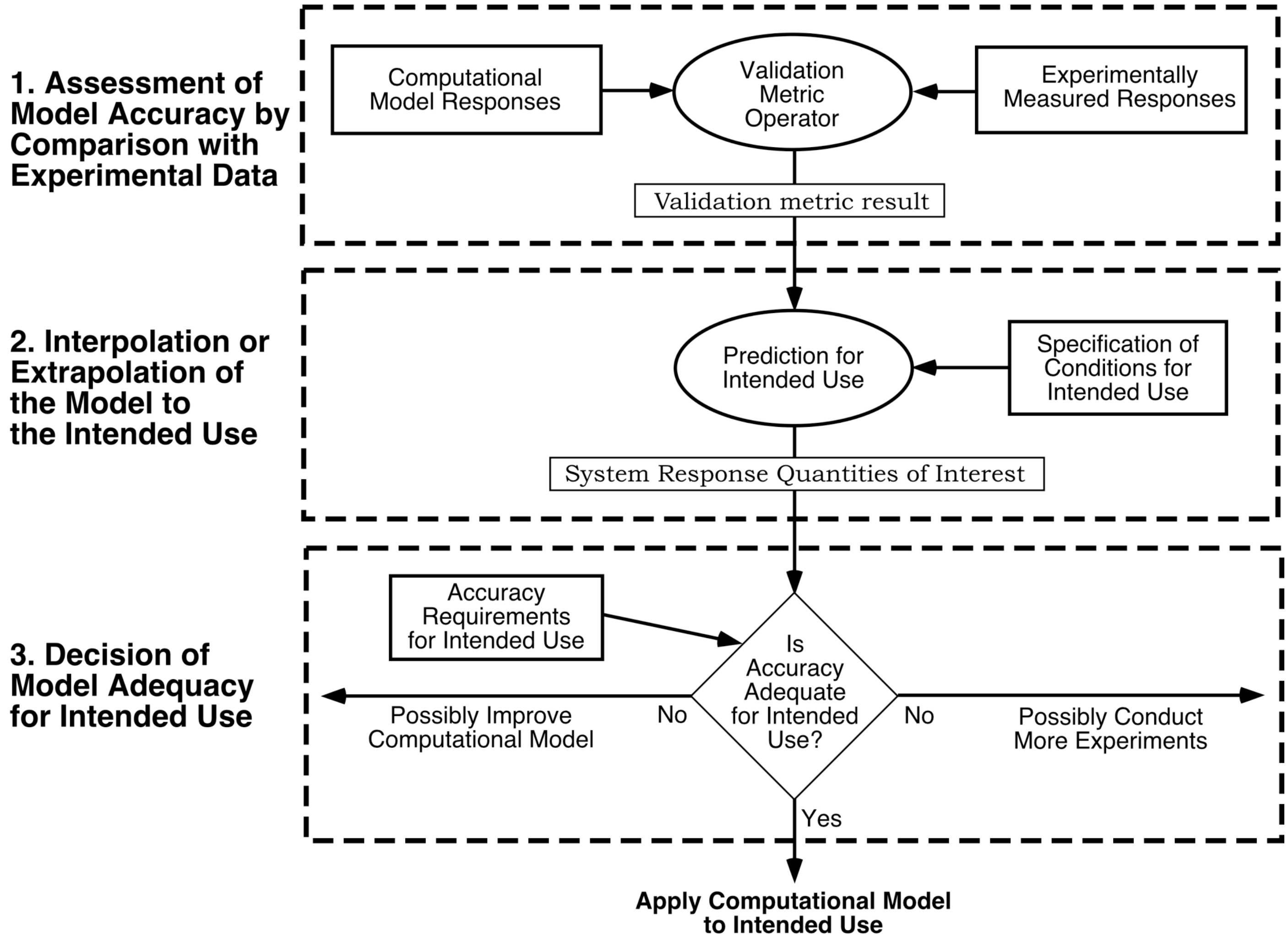
- CSE development of V&V methodology and practices:
  - American Institute of Aeronautics and Astronautics published the first engineering standards document on V&V: "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations," American Institute of Aeronautics and Astronautics, AIAA-G-077-1998.
  - American Society of Mechanical Engineers published a recent engineering standard: "Guide for Verification and Validation in Computational Solid Mechanics," ASME V&V 10-2006."
- Important difference in validation methodology between DoD and CSE:

Validation can only be conducted by comparison with experimentally measured data.

ASME Validation Procedure

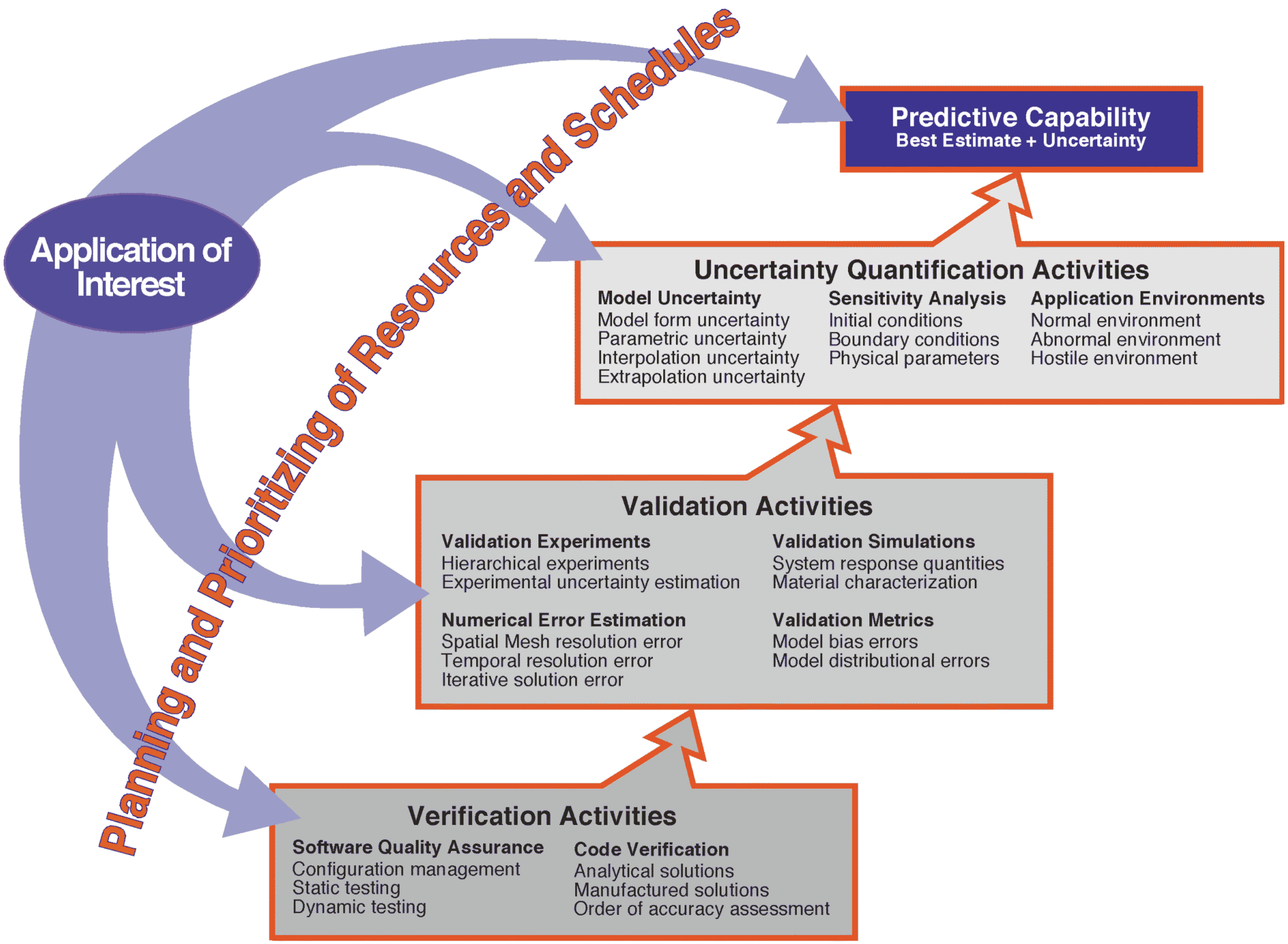


Three Aspects of Validation



(Ref: Oberkampf and Trucano, 2007)

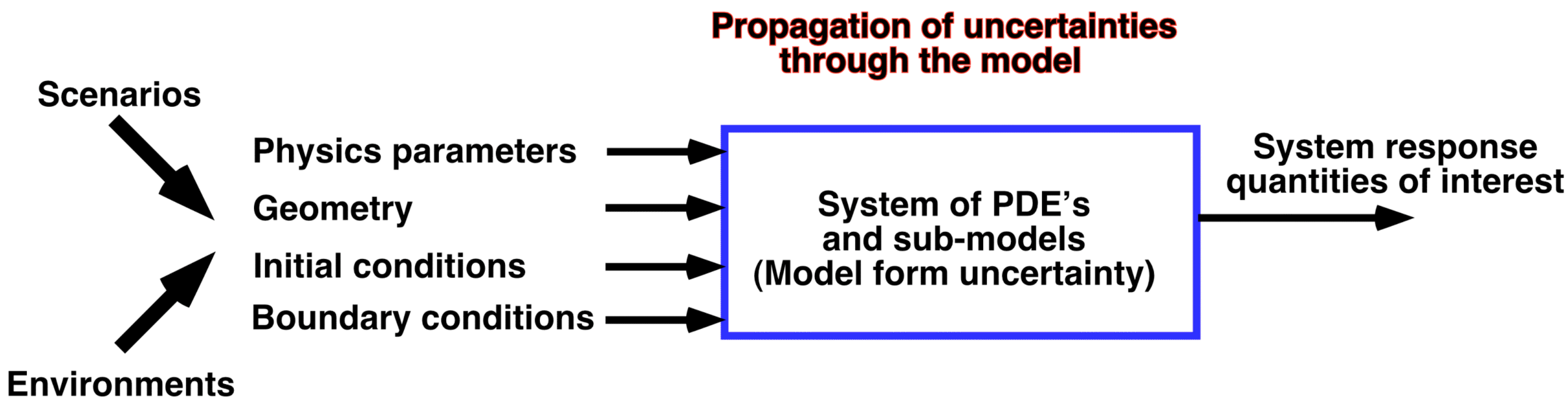
Elements of Predictive Capability



Recognition of Different Types of Uncertainty

- **Aleatory uncertainty** is an inherent variation associated with the physical system or the environment
  - Also referred to as variability, irreducible uncertainty, and stochastic uncertainty, random uncertainty
- Examples:
  - Variation in weather conditions
  - Variation in manufacturing and assembly of systems
- **Epistemic uncertainty** is an uncertainty that is due to a lack of knowledge of quantities or processes of the system or the environment
  - Also referred to as subjective uncertainty, reducible uncertainty, and model form uncertainty
- Examples:
  - Lack of experimental data to characterize new materials and processes
  - Poor understanding of physics phenomena
  - Lack of experimental data/testing for complete systems

Propagation of Uncertainties



The propagation of uncertain input quantities through a mathematical model to obtain outputs can be written as

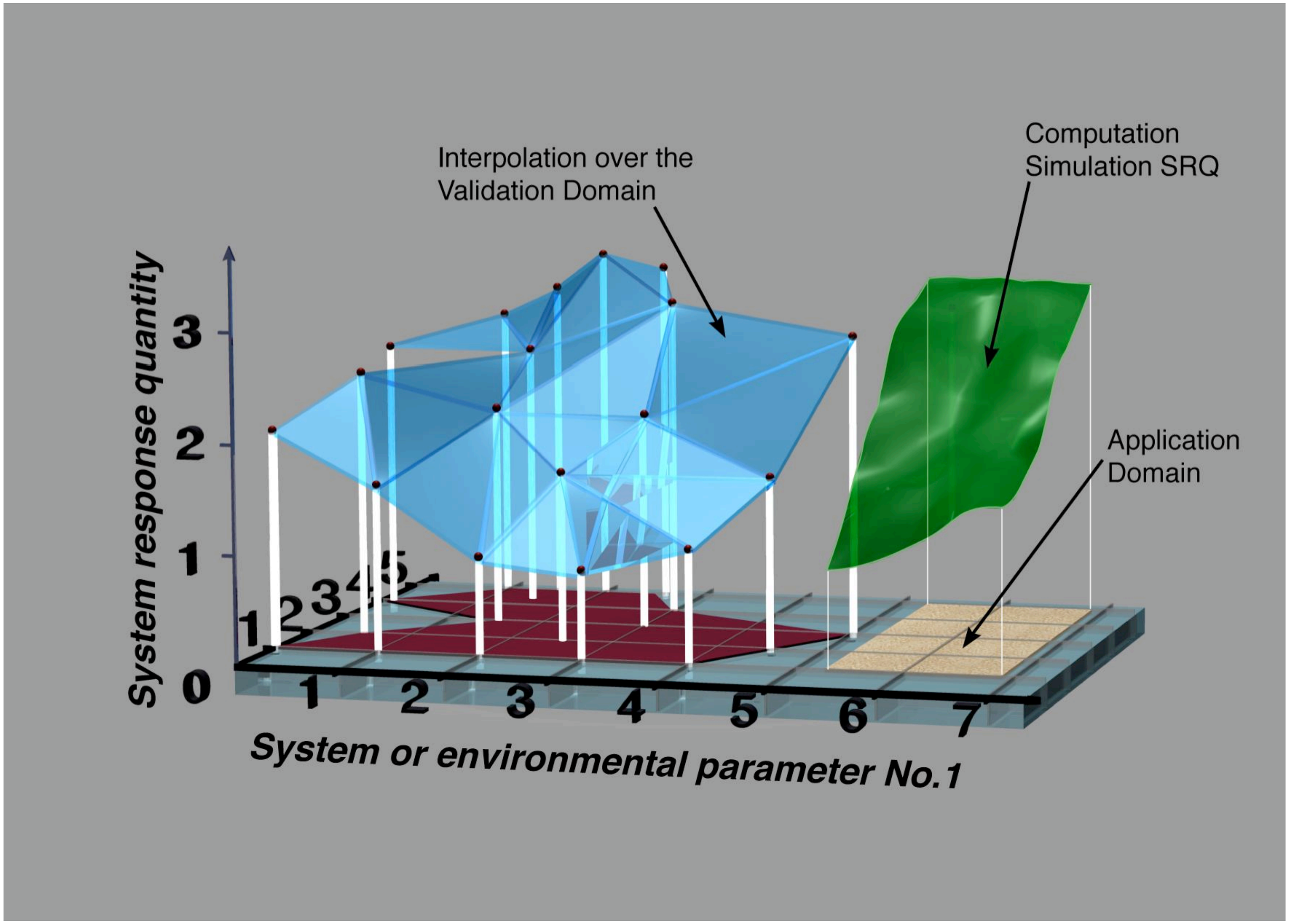
$$y = f(\vec{x}_a, \vec{x}_e)$$

- y **is a system response quantity of interest**
- f **is the mathematical model of the physical process of interest**
- $\vec{x}_a = x_1, x_2, \cdots x_m$ **is the vector of all aleatory uncertainties**
- $\vec{x}_e = x_{m+1}, x_{m+2}, \cdots x_n$ **is the vector of all epistemic uncertainties**

Methods for Propagating Aleatory and Epistemic Uncertainties

- **Second-order probabilistic analysis:**
  - Use a two step process separating epistemic and aleatory uncertainties
  - Treat the range all epistemic uncertainties as possible realizations with no probability associated with realizations from sampling
  - Treat aleatory uncertainties as random variables
- **Robust Bayesian inference:**
  - Investigate the effect of different assumptions of prior distributions
  - Investigate the effect of partitioning the available data
- **Evidence theory:**
  - Can represent aleatory and epistemic uncertainties within one framework
  - Early criticism misdirected at Dempster's rule of aggregation of evidence
  - Early applications have been very successful

Key Area of Concern: Large Extrapolation of the Model



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Closing Remarks

- V&V program in ASC has made significant contributions to:
  - Code and solution verification
  - Methodology for the design and execution of validation experiments
  - Distinction between calibration and validation of models
  - Statistical methods for accuracy assessment of models
  - Uncertainty quantification of predictive capability
- Improved credibility in M&S can only be achieved through improved procedures and consistent application of V&V&UQ
- Diverse challenges:
  - Technical
  - Cultural

Goal: Improved Risk-Informed Decision Making for the Stockpile