Validation and Calibration in a Design Environment

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Outline of the Presentation

- Steps in the design process
- Approaches to model prediction
- Critical research areas

Steps in the Design Process

- **Specify the conditions of the application domain:**
  - Determine if an existing computational model is appropriate to use
  - Determine initial conditions, boundary conditions, excitation conditions, etc
- **Compare the application domain to previous uses of the model:**
  - Determine maturity of the CAD/CAM model, SQA, code verification, etc
  - Estimate model accuracy based on previous uses of the model (validation)
- **Identify, characterize, and calibrate the uncertainties:**
  - Determine and characterize uncertainties in operating conditions, ICs, BCs, excitation conditions, material properties, model extrapolation, etc
  - Calibrate parametric uncertainties based on available experimental data
- **Conduct sensitivity analyses and tradeoff studies:**
  - Conduct global sensitivity analyses on system response quantities of interest
  - Conduct tradeoff studies of design parameters and operating conditions, including time and resource requirements
- **Present simulation results to decision makers:**
  - Present design tradeoffs, explicitly including uncertainties and risks
  - Make design decisions, including risk reduction and contingency plans

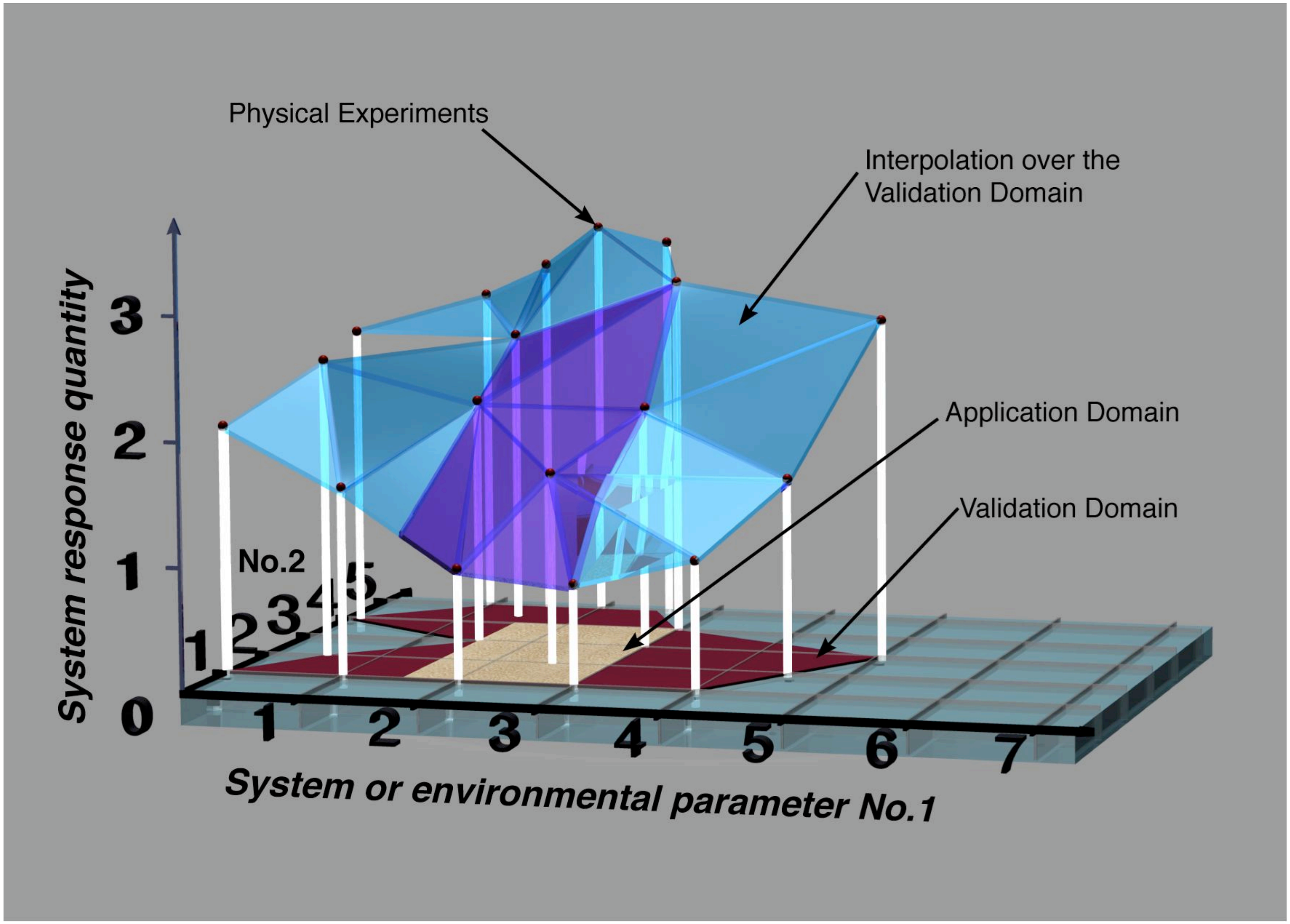
Approaches to Model Prediction

- **Traditional Bayesian calibration of the model:**
  - Assume all parameters are random variables
  - Assume prior distributions for uncertain parameters
  - Update the prior distributions for uncertain parameters using available experimental data and Bayes formula
  - Use the updated parameter distributions in the model to make predictions for the application of interest
  - Disadvantages:
    - Assumes the key issue is calibrating parameter distributions
    - Assumes the model form is accurate
    - Is computational very expensive
- **Approach of Kennedy and O'Hagan (2001)**
  - Attempts to segregate parameter updating and model form uncertainty estimation

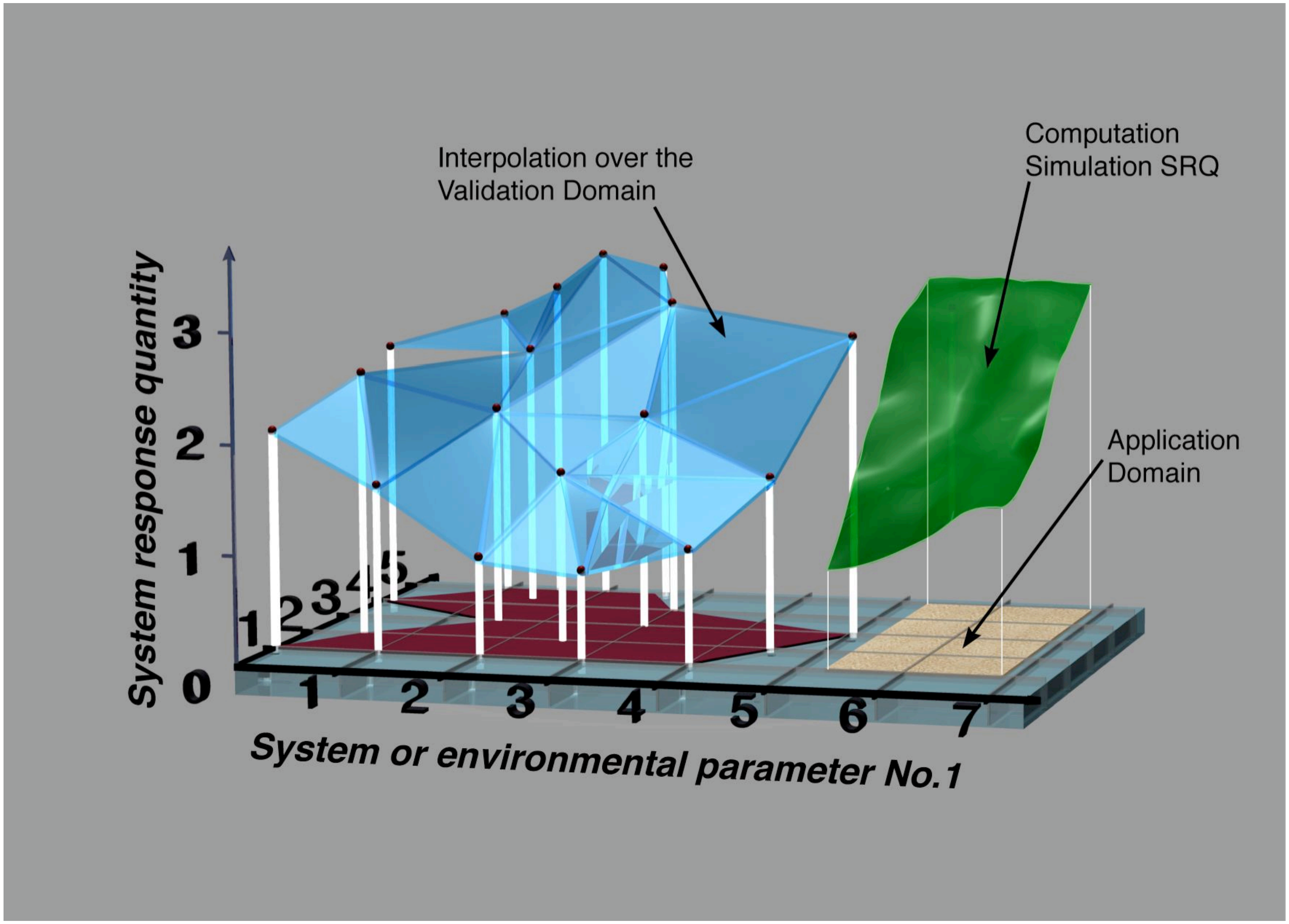
Alternative Approach to Model Prediction

- Characterize all of the uncertainties:
  - Aleatory: random variability associated with the parameter
  - Epistemic: uncertainty due to lack of knowledge
- Calibrate uncertain model parameter distributions before model validation or prediction activities
- Assess the model accuracy by quantitative comparisons with experimental validation data, i.e., compute a validation metric
- Use the model to make predictions for the application domain:
  - Use either second order probability or evidence theory to propagate uncertainties through the model
  - Model-form inaccuracies are treated as an epistemic uncertainty
  - Extrapolate the model form uncertainty to the application domain
- Advantages over Bayesian approaches:
  - Better able to estimate model uncertainty
  - Better able to deal with little experimental data
  - More appropriate for large extrapolations of the model

Typical Application of a Model: Interpolation



Large Extrapolation of a Model



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Critical Research Areas in Predictive Simulation

- **Improvements needed in Bayesian inference:**
  - **Better methods to separate parameter distribution updating from estimating model form error**
  - **Better methods to estimate uncertainty in updated models**
- **Improvements needed in the alternative approach:**
  - **Better methods to extrapolate a validation metric to the application domain**
  - **Better methods to estimate model form error due to large extrapolations of the model**

Goal: Better capture uncertainty in our predictions for the decision maker