# Perspectives on Verification, Validation, and Uncertainty Quantification


**William L. Oberkampf, PhD**

**Consultant**
**Albuquerque, New Mexico**
**wloconsulting@gmail.com**



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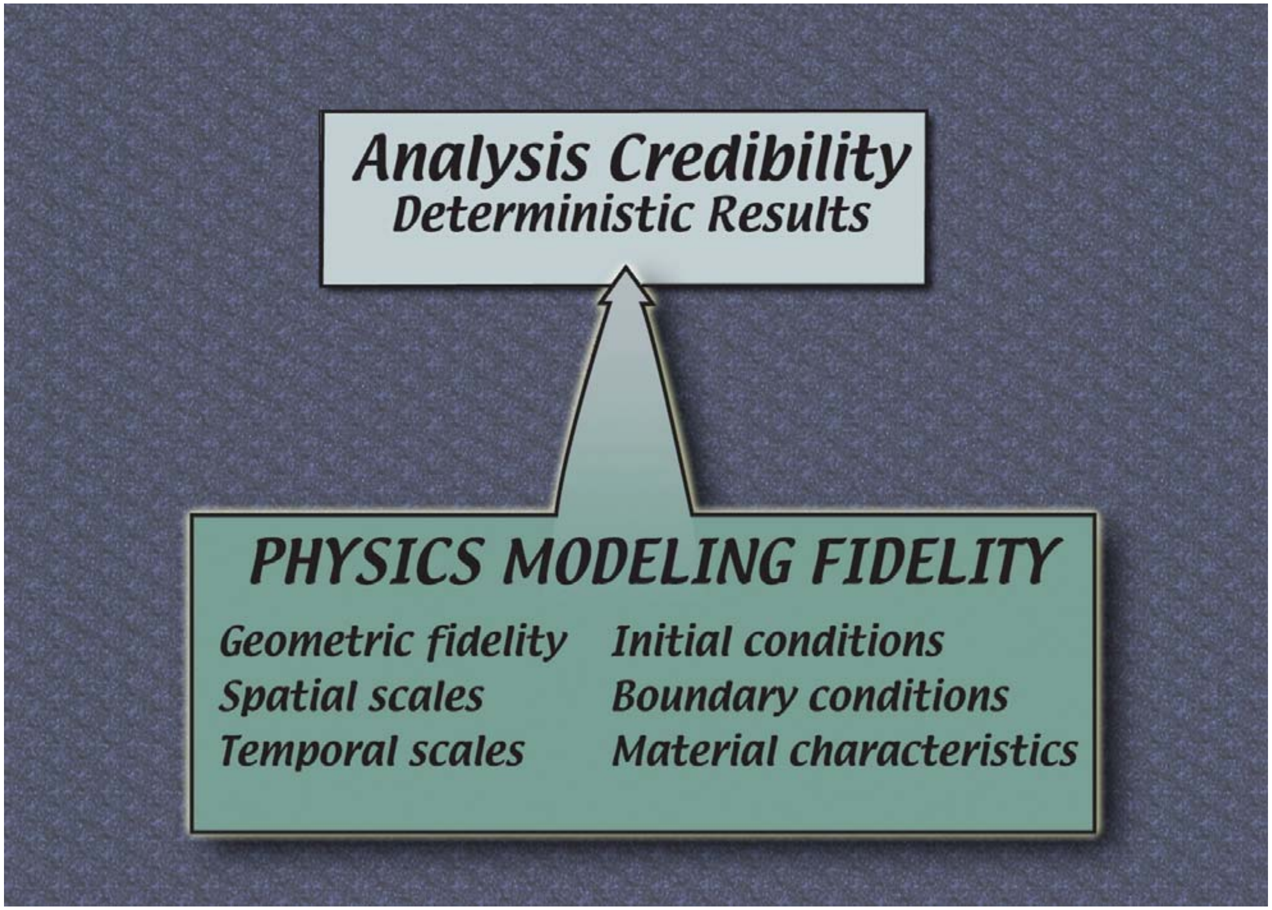
# Outline of the Presentation

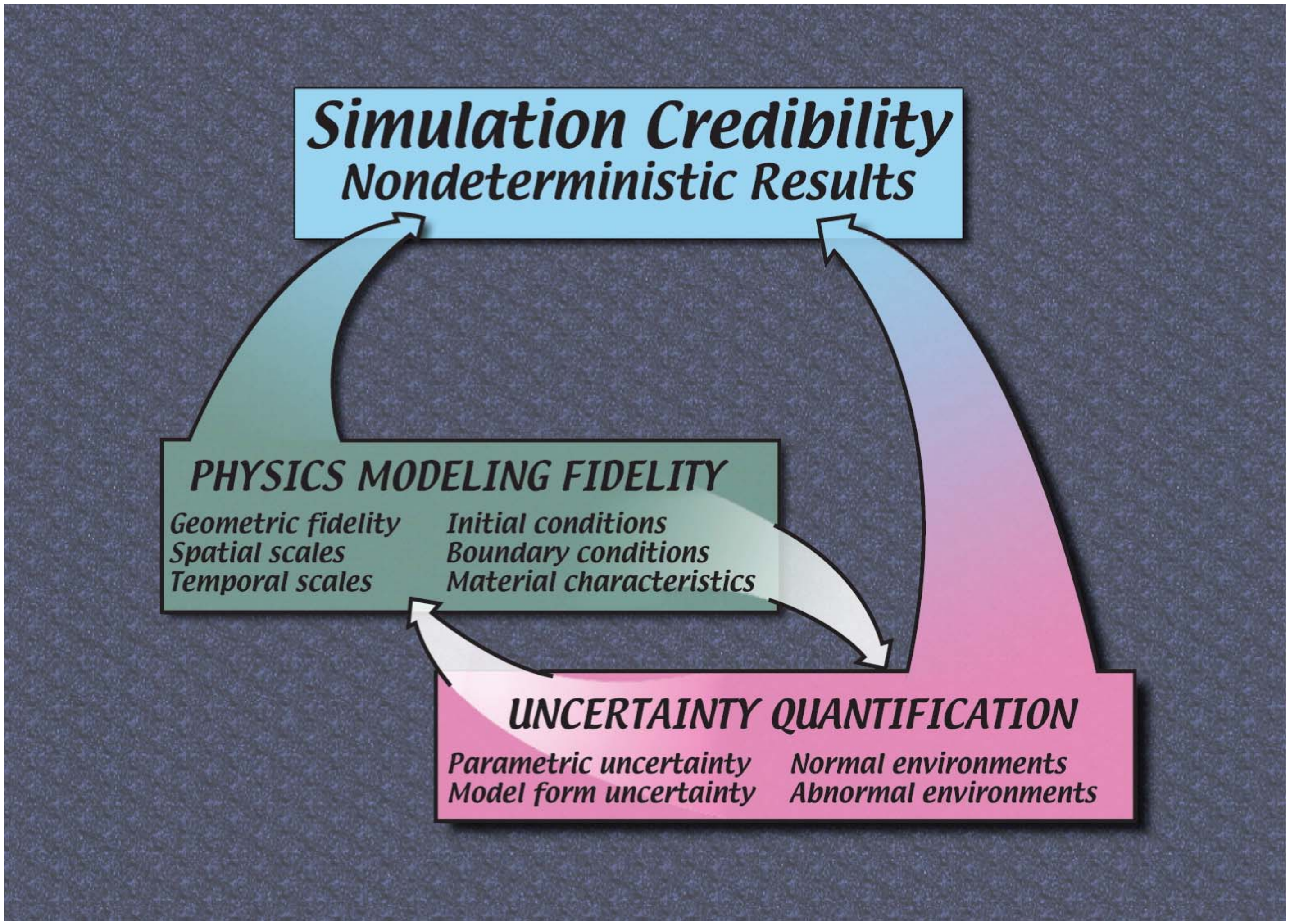
- Uses of computational simulation
- Verification, validation and uncertainty quantification
- Where do we stand?
- Research and implementation issues
- Closing Remarks

**Work in collaboration with Tim Trucano and Martin Pilch, Sandia Nat'l. Labs., and Scott Ferson and Jon Helton, consultants.**

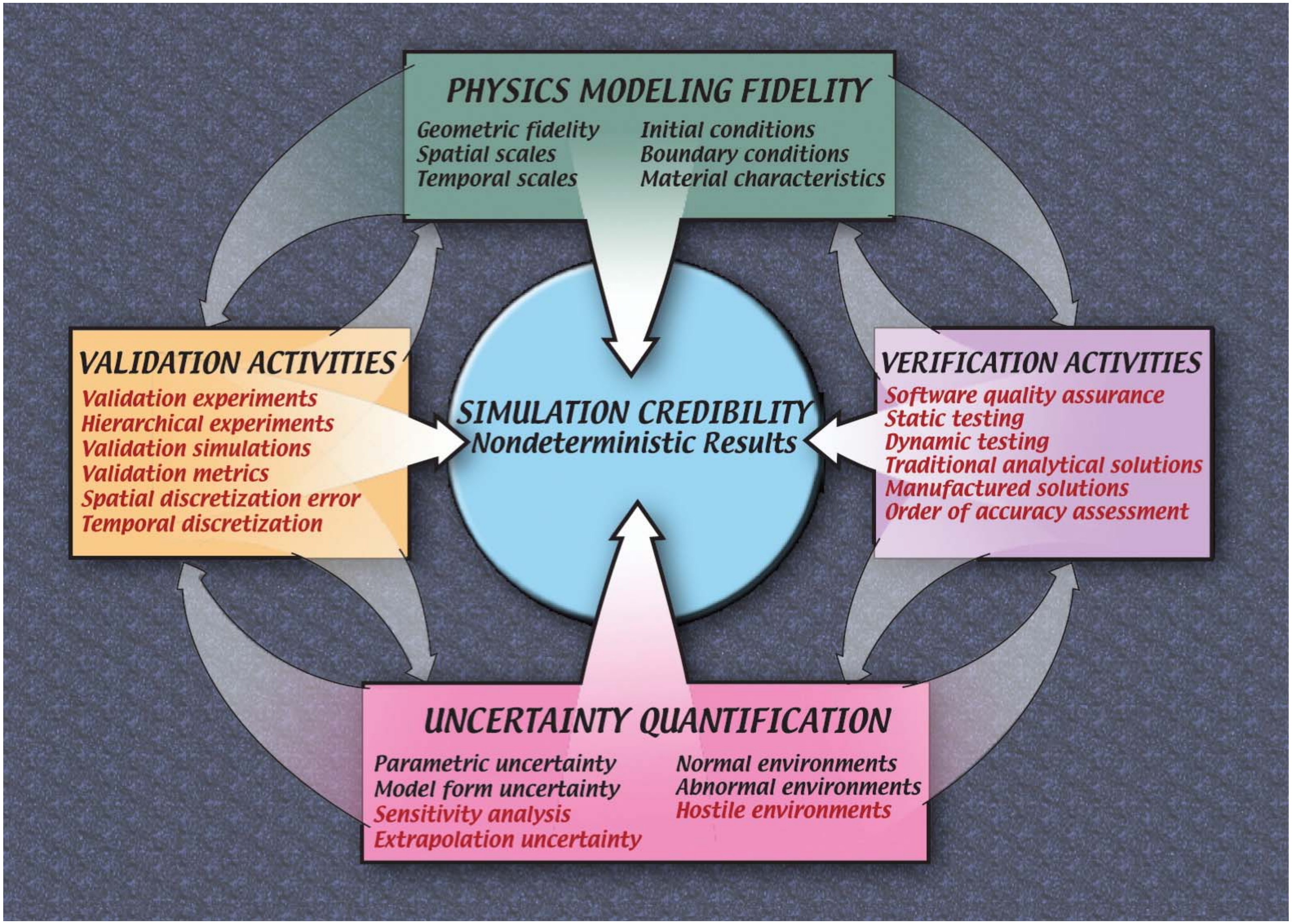
# Typical Research Activity in Computational Science and Engineering



# Uncertainty Quantification Included in Analyses for Decision Making



# Verification and Validation Included in High-Consequence Decision Making



# Verification Activities

- Definition used by U.S. DoD, AIAA, and ASME:

  **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.

- Two elements of verification are well recognized:
- **Code Verification**: Verification activities directed toward:
  - Finding and removing mistakes in the source code
  - Finding and removing errors or weaknesses in the numerical algorithms
  - Improved software reliability using software quality assurance practices
- **Solution Verification**: Verification activities directed toward:
  - Assuring the appropriateness of input and output data for the problem of interest
  - Estimating the numerical solution error, e.g. error due to finite element mesh resolution and time discretization

# Validation Activities

- **Definition used by U.S. DoD, AIAA, and ASME:**

  **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**

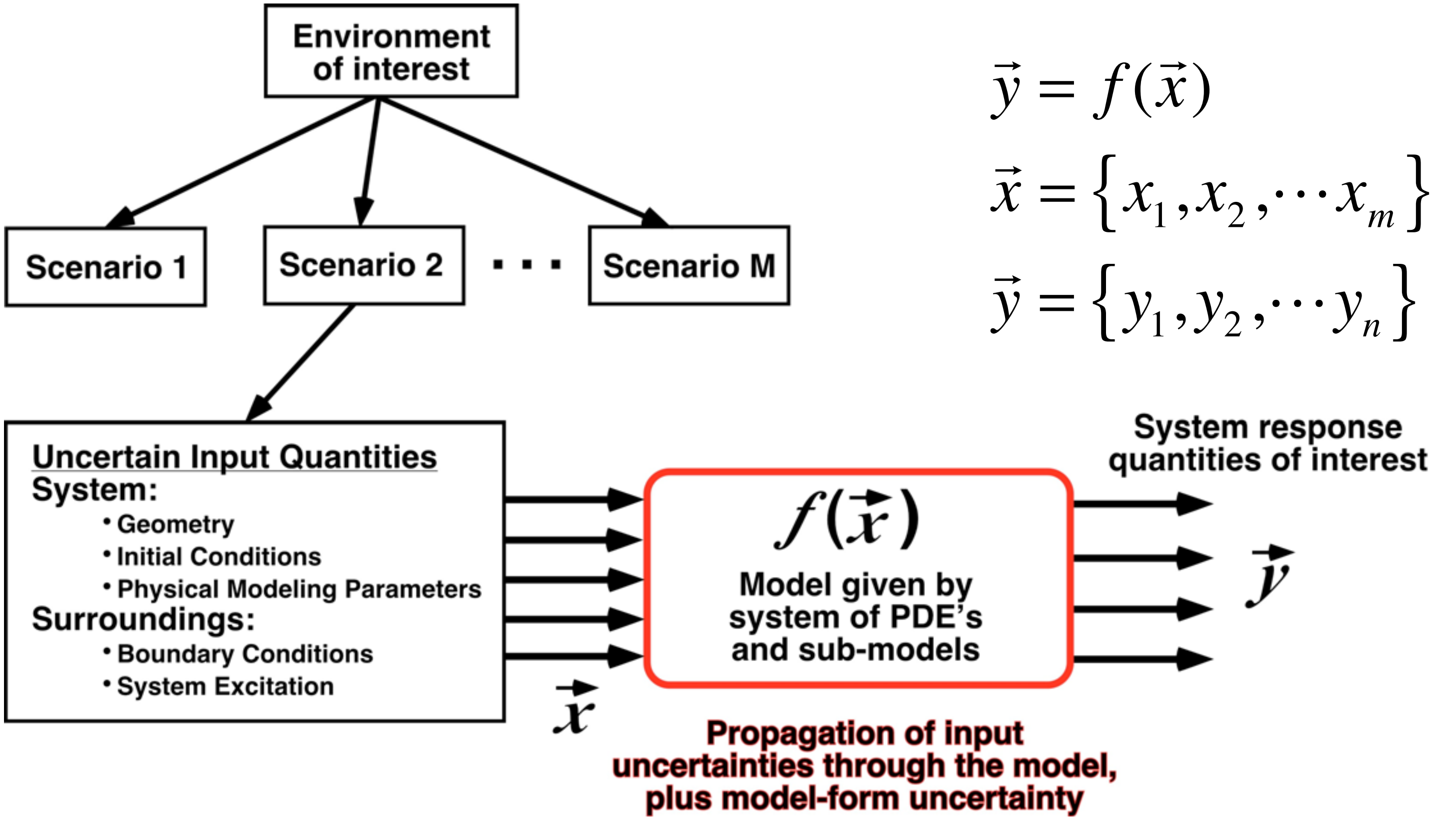
- **Validation is concerned with three activities:**
  - **Model accuracy assessment by comparison with a referent**
  - **Application of the model to the intended use, e.g., conditions where no referent data exist**
  - **Decision of model adequacy for the intended use**

- **Engineering and science communities require that the referent be experimentally measured data**

- **DoD allows any reasonable referent**

- **IEEE and ISO use different definitions of V&V, but they can be viewed as more general definitions**

# Uncertainty Quantification Activities




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

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

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

- **Key sources of uncertainty:**
  - **Identification of environments and scenarios of the system**
  - **Input uncertainties in the system and in the surroundings**
  - **Model form uncertainty, i.e., uncertainty in *f*(•)**

# Where Do We Stand?
# Verification Activities

- **Code verification:**
  - **Some commercial codes have extensive test suites composed of traditional analytical solutions**
  - **Weaknesses with code testing:**
    - **Traditional analytical solutions do not test complex coupling of terms**
    - **Order-or-accuracy testing is not done**
  - **Government, corporate, and university code testing is spotty, at best**
- **Software quality assurance (Hatton, 1997):**

  **"Scientific calculations should be treated with the same measure of disbelief researchers have for unconfirmed physical experiments."**

- **Solution verification:**
  - **Error estimation usually relies on experience of the analyst, instead of quantitative error estimation**
  - **If model predictions agree with experimental data, there is little enthusiasm for investigating possible numerical errors**
  - **Sometimes it is fully recognized that numerical errors are as large as physics modeling errors, so model parameters are calibrated to adjust**

# 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 so that the model agrees with the experimental data
  - Usually reliable when the models are used for very similar systems and conditions where the models are calibrated
  - Weaknesses in the models, or coding errors, are rarely uncovered
- A relatively new approach to validation:
  - Emphasis is on assessment of model prediction inaccuracy, in the sense of a blind-prediction
  - Quantitative measures of disagreement (validation metrics) are assessed between model predictions and experimental measurements
  - More reliable when using the model to predict system responses:
    - Far from the conditions of the validation experiments
    - When the complete system can not be tested

# Where Do We Stand: Uncertainty Quantification Activities

- Approach used in most high-consequence systems:
  - Characterize all uncertainties as either aleatory or epistemic:
    - Aleatory: inherent variation associated with the quantity, represented as a probability distribution
    - Epistemic: uncertainty due to lack of knowledge of the quantity, represented as an interval
  - Propagate input uncertainties through the model using Monte Carlo sampling techniques
  - Use alternate models to investigate model form uncertainty
- Bayesian approach:
  - Assume prior distributions for uncertain parameters in the model
  - Update the prior distributions for uncertain parameters using available experimental data an Bayes formula
  - Use Monte Carlo sampling, MCMC, or construct surrogate models to propagate uncertainties and update prior distributions
  - Compute new predictions using updated parameter distributions

# Research and Implementation Issues: Verification Activities

- **Develop manufactured solutions for a wide range of physics and engineering disciplines for order of accuracy testing**
- **Develop improved measures of code coverage in testing software; line coverage in regression testing is inadequate**
- **Develop less expensive and more robust methods for estimating spatial and temporal discretization error**
- **Develop numerical error estimators for nonlinear parabolic and hyperbolic PDEs**
- **Require improved code verification evidence from code developers**

**“I’ve already refined the mesh**

**down to the microstructure of the metal!”**

# Research and Implementation Issues: Validation Activities

- Improve coordination and synergism between experimentalists and computationalists in designing and executing validation experiments
- Develop consortia to share validation test data among industry, commercial software companies, government, and universities
- Develop improved validation metrics to deal with:
  - Epistemic uncertainty in either the model or the experiment
  - Time series analysis
- Using the Bayesian updating approach, improve the separation of parameter updating and model error estimation

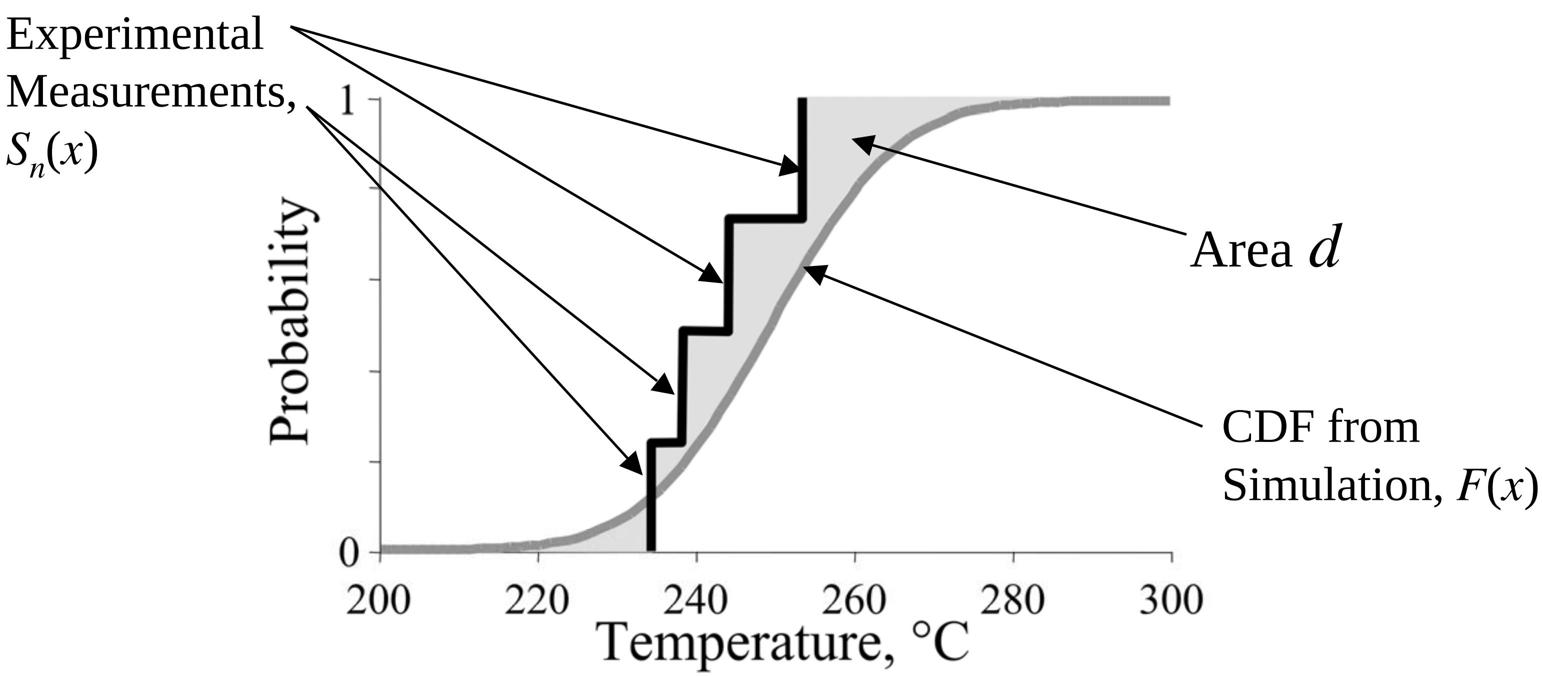
**"Our results agree with the experimental data,**

**why are you being difficult?"**

# Area Validation Metric

- **The validation metric is defined to be the area between the CDF from the simulation and the empirical distribution function (EDF) from the experiment**

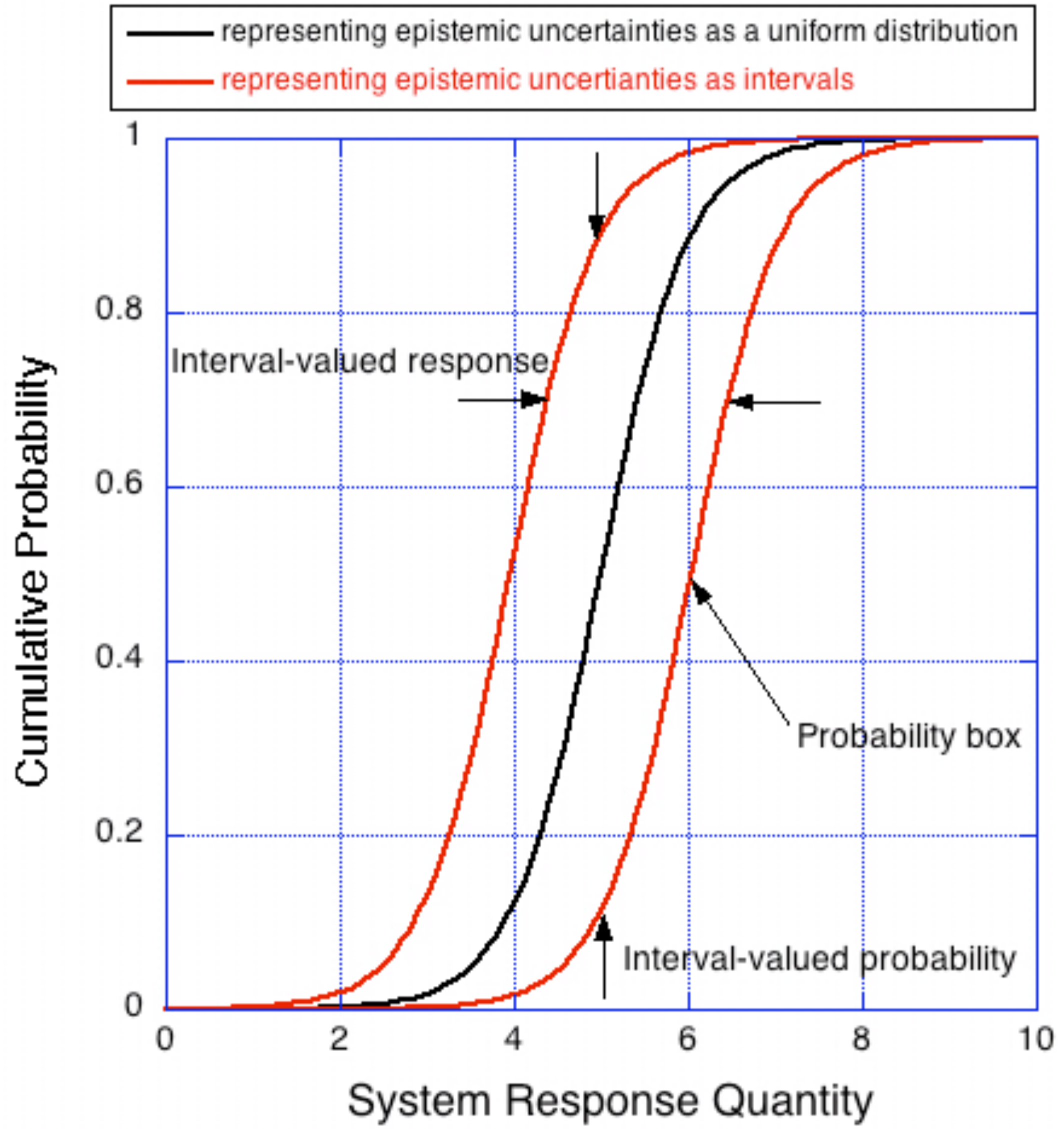
$$d(F, S_n) = \int_{-\infty}^{\infty} \left| F(x) - S_n(x) \right| \mathrm{d}x \qquad \text{(Minkowski } L_1 \text{ metric)}$$



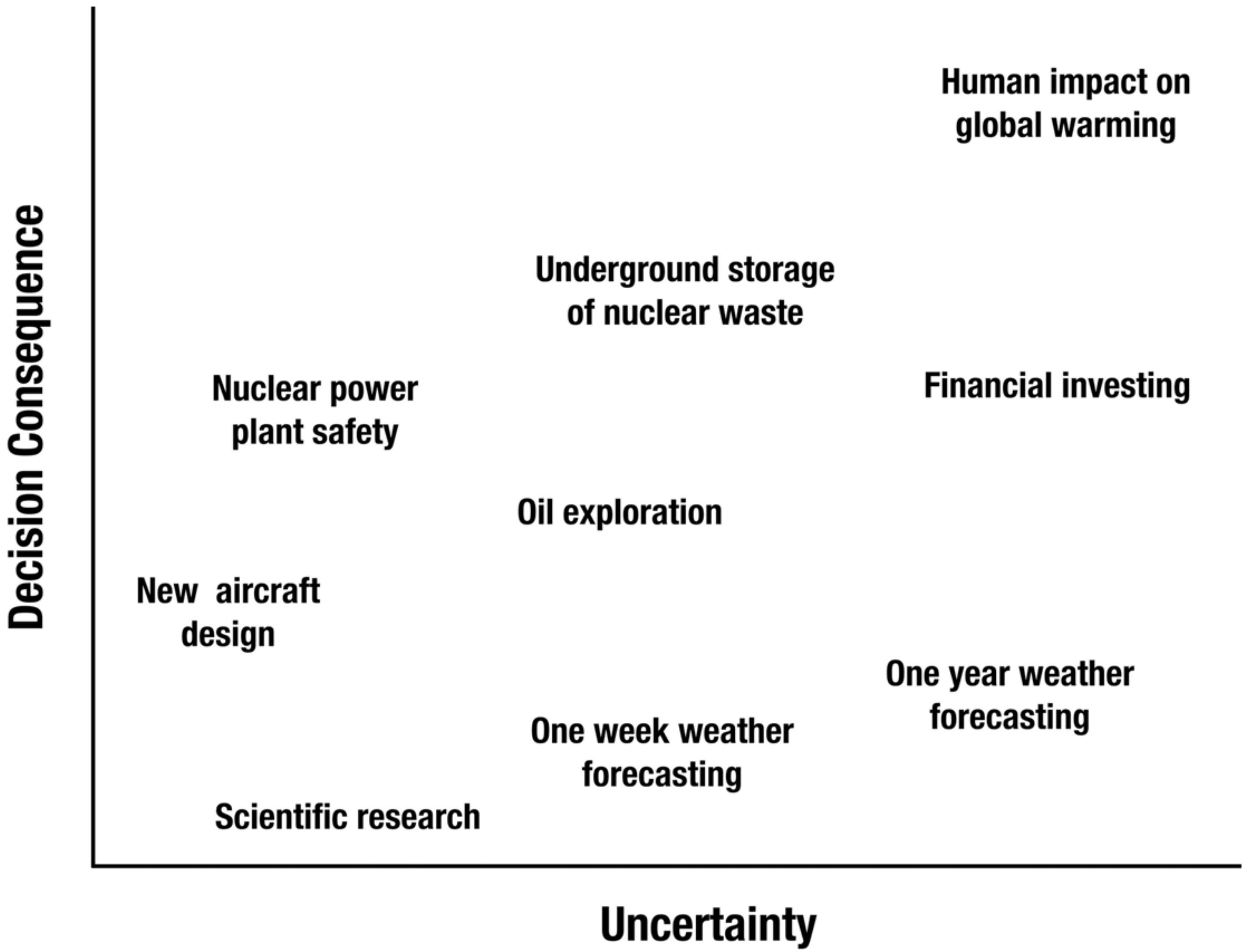
# Research and Implementation Issues: Uncertainty Quantification Activities

- **Improve the recognition and interpretation of aleatory and epistemic uncertainty**
- **Conduct further research and application of:**
  - **Probability bounds analysis (second order analysis)**
  - **Evidence theory (Dempster-Shafer theory)**
- **Extend Bayesian methods and polynomial chaos methods to incorporate interval-valued quantities**
- **Develop improved methods for estimating the change in model form uncertainty due to extrapolation:**
  - **Construct a non-Euclidian space for extrapolation**
  - **Map system response quantities to a probability space and then use the model prediction as an inverse transform to return to physical space**
- **Develop improved methods for sensitivity analysis when uncertainties are both aleatory and epistemic in nature**

# Effect of Characterizing Epistemic Uncertainties as Intervals versus Uniform Distributions



# Risk-Informed Decision Making



# Closing Remarks

- **Verification and validation are processes that develop evidence of credibility in simulations**
- **Uncertainty quantification should forthrightly estimate:**
  - **Uncertainty associated with identified environments and scenarios**
  - **Uncertainty in simulation input quantities**
  - **Uncertainty in the model form applied at the conditions of interest**
- **What can be learned from failures in computational simulation?**
  - **Weaknesses in identifying failure modes**
  - **Under estimation of both aleatory and epistemic uncertainty**
  - **Inadequate quantification of model form uncertainty**
  - **Ability of decision makers to influence the analysis outcomes**

**V&V&UQ are concerned with truth in simulation, not marketing.**

- **We must recognize that engineering analysis, and how it is coupled to decision making, has fundamentally changed.**

# Some Prefer to Take the Position

**“I don’t have the time, money, or people to do V&V&UQ.”**

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wloconsulting@gmail.com

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