



Model Validation under Both Aleatory and Epistemic Uncertainty

William L. Oberkamp

Distinguished Member Technical Staff
Validation and Uncertainty Quantification Department
Sandia National Laboratories, Albuquerque, New Mexico
wloberk@sandia.gov

Scott Ferson

Applied Biomathematics
100 North Country Road
Setauket, New York
scott@ramas.com

NATO/RTO Applied Vehicle Technology Panel
Symposium on Computational Uncertainty in Military Vehicle Design
Athens, Greece
3-6 December 2007



Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.





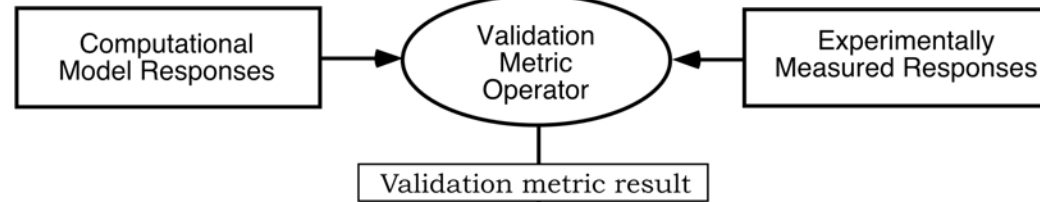
Outline of the Presentation

- **Background**
- **Need for a new approach**
- **Area validation metric**
- **Pooling of incomparable comparisons**
- **Aleatory and epistemic uncertainty**
- **Closing remarks**

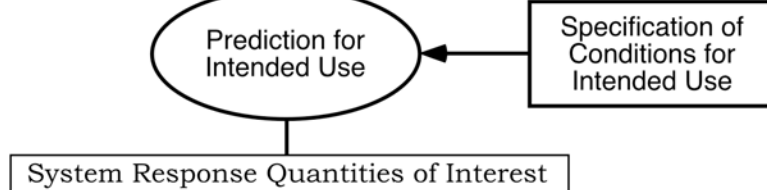


Background: Aspects of Validation

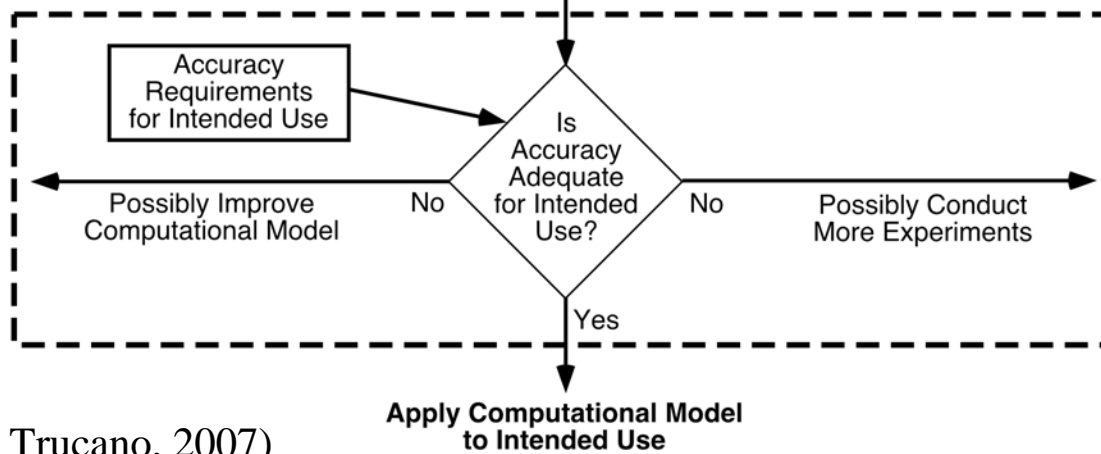
1. Assessment of Model Accuracy by Comparison with Experimental Data



2. Interpolation or Extrapolation of the Model to the Intended Use



3. Decision of Model Adequacy for Intended Use



(Oberkampf and Trucano, 2007)



Review of Existing Approaches

- **Comparison of mean value from simulation and experiment**
 - Only measures the mismatch between simulation and experiment at the expected value
- **Hypothesis testing**
 - Measures the mismatch between probability distributions from simulation and experiment
 - Mismatch is measured by a probability value
- **Bayesian validation**
 - Focused on evaluating a subjective probability that a simulation is consistent with experiment
 - Emphasis is on updating probability density functions of uncertain parameters to obtain best agreement with experiment
 - Assumes the model form is correct



Need for a New Approach

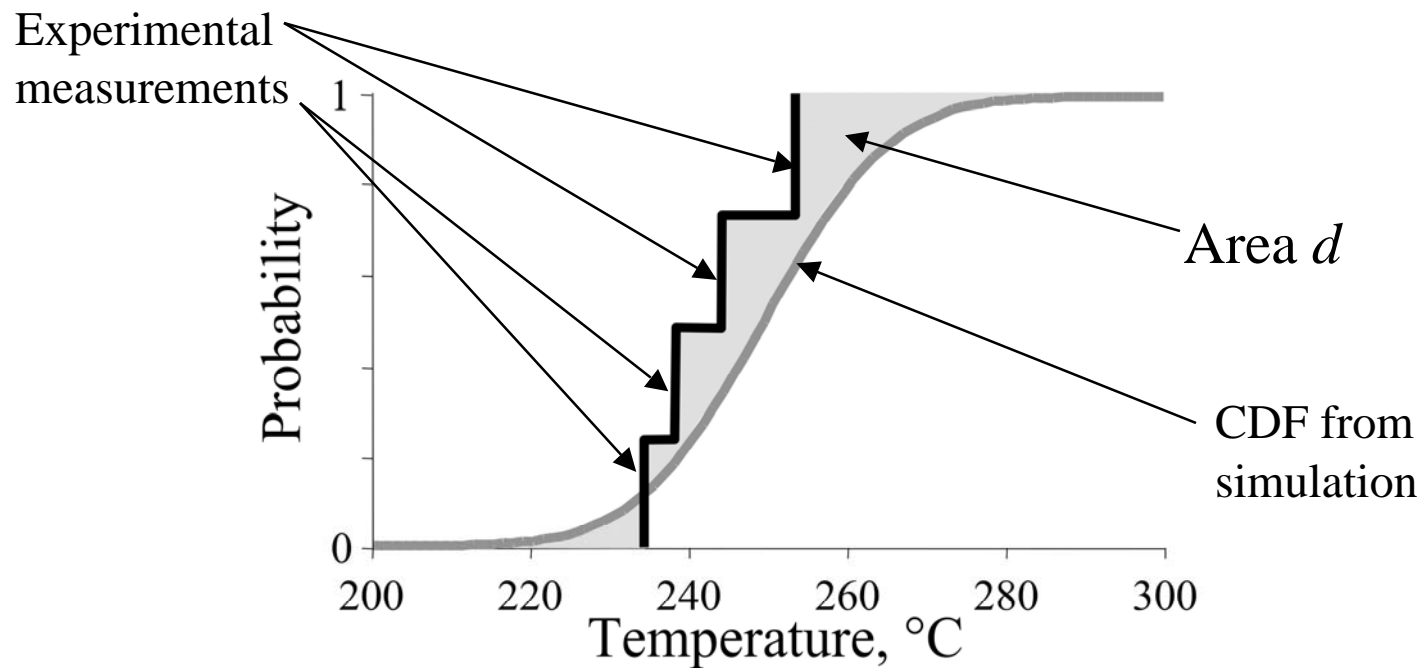
- **Our validation metric approach emphasizes:**
 - Objectively measuring mismatch between cumulative distribution functions (CDFs) between simulation and experiment
 - Quantifying model form uncertainty, in the spirit of a “blind” comparison with experiment
 - Estimating the mismatch in terms of the units of the system response quantity (SRQ) being compared
- **Our approach can address:**
 - Comparison between simulation and experiment with as few as one sample each
 - Pooling of comparisons from dissimilar system response quantities
 - Epistemic uncertainty existing either (or both) the simulation and the experimental measurements



Area Validation Metric

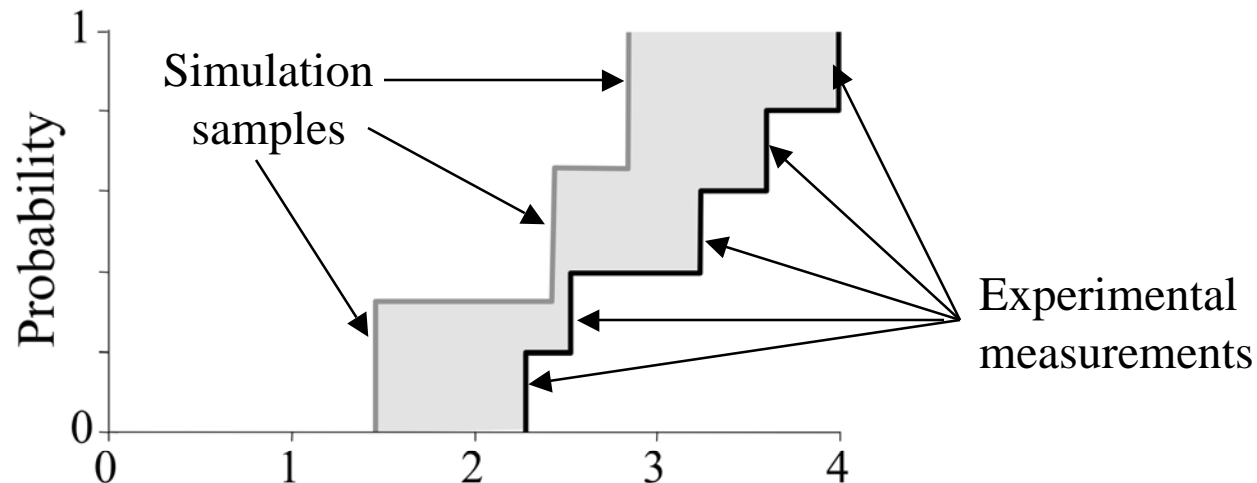
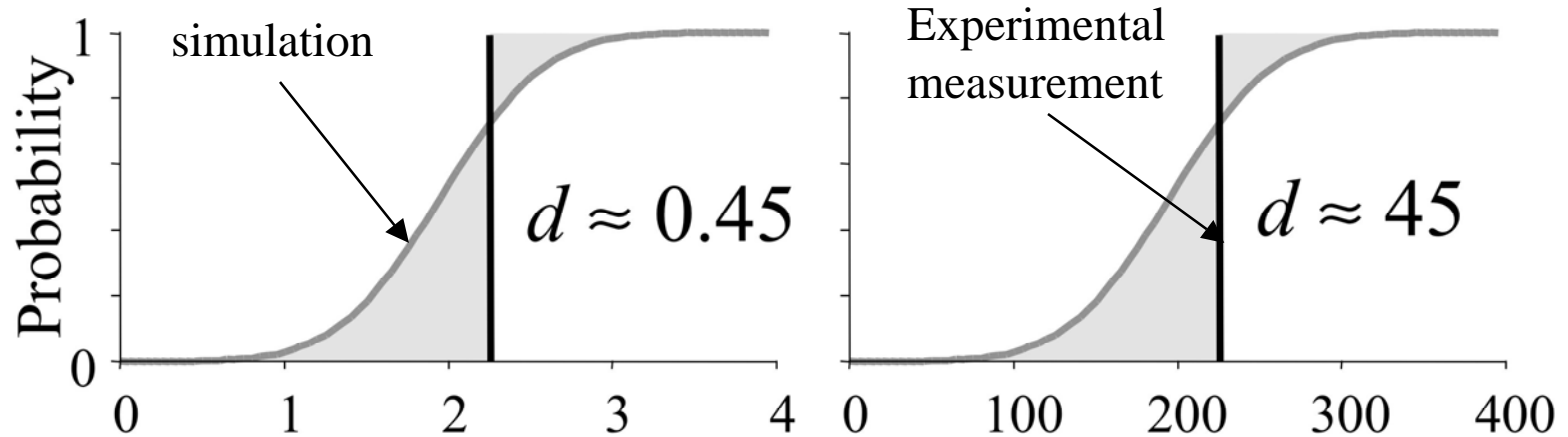
- The validation metric is defined to be the area between the cumulative distribution function (CDF) from the simulation and the empirical distribution function (EDF) from experiment (Minkowski L_1 metric)

$$d(F, S_n) = \int_{-\infty}^{\infty} |F(x) - S_n(x)| dx$$





Area Validation Metric (from Ferson et al 2008)



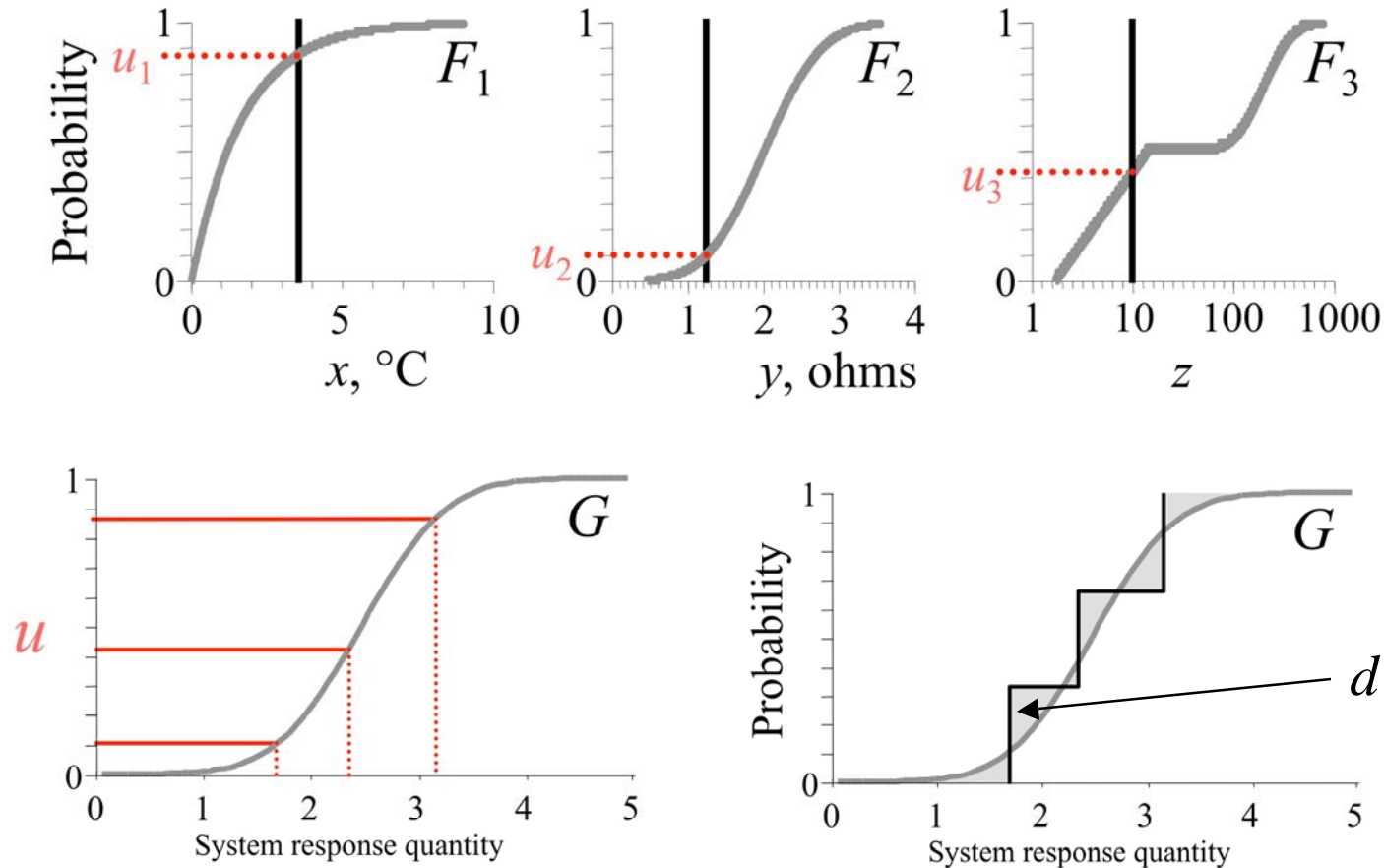


How can Different Validation Metric Results be Combined?

- Two common situations in comparison of simulation and experiment:
 - We have a time dependent SRQ and we have computed individual validation metrics at several instances of time
 - We have computed a validation metric for different SRQs
- Instead of using the probability integral transform theorem (Angus, 1994) in the forward direction
- Given a distribution F and a uniform random variable u between zero and one, the value of $F^{-1}(u)$ will be a random variable distributed according to F .
- We can:
 - Use it to back-transform from individual SRQs (physical space) to a probability space.
 - Then use an appropriate CDF, for the problem of interest, to transform back into physical space so that a validation metric can be computed.



Pooling of Incomparable Comparisons





Aleatory and Epistemic Uncertainty

- **Aleatory uncertainty** is an inherent variation associated with a parameter, physical system, or environment
 - Also referred to as variability, stochastic uncertainty, irreducible uncertainty
- **Examples:**
 - Variability in geometric parameters due to manufacturing
 - Variability in weather conditions
- **Epistemic uncertainty** arises from imperfect knowledge or ignorance
 - Also referred to as subjective uncertainty, reducible uncertainty, or model form uncertainty
- **Examples:**
 - Insufficient experimental data to precisely characterize a probability distribution
 - Poor understanding of physics phenomena or physics coupling
 - Poor understanding of failure modes or hostile environments



Measurement Uncertainty

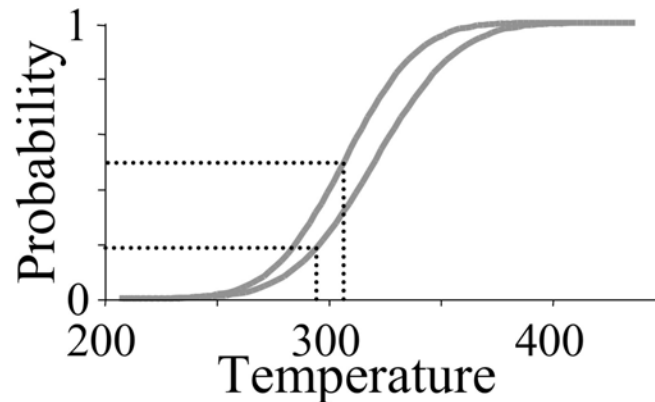
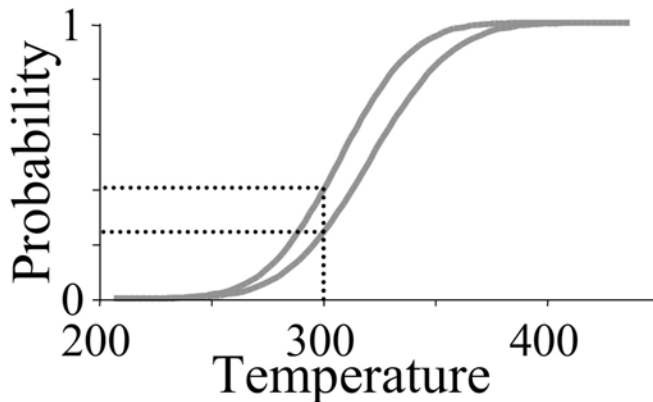
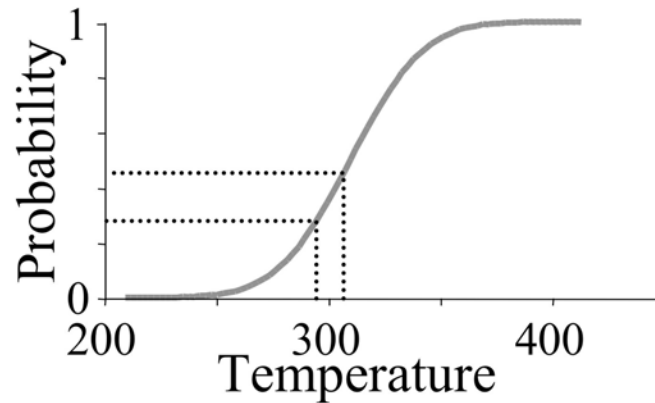
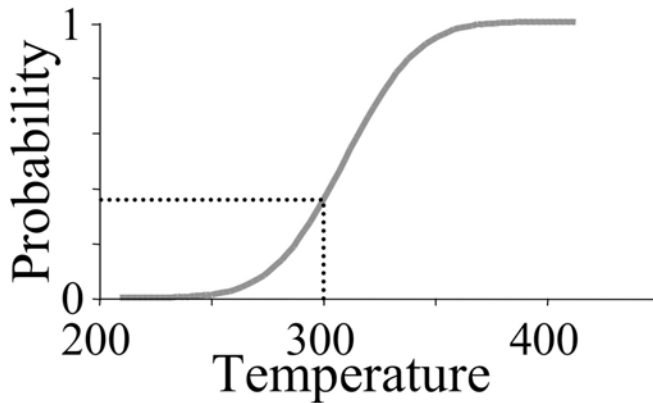
- Traditional ISO/NIST approach is focused on the estimation of random measurement uncertainty of a fixed quantity.

$$Y = X + \varepsilon$$

- X is the true, but unknown, value of the measurand
 - ε is the random measurement error
 - Y is measured value
- Using either higher accuracy measurements or repeated measurements of X , ε is characterized as a parametric probability distribution along with its parameters.
 - Recent work by Ferson et al (2007) developed methods for estimating epistemic uncertainty in measurements, e.g., due to:
 - Data censoring
 - Missing values
 - Sampling uncertainty

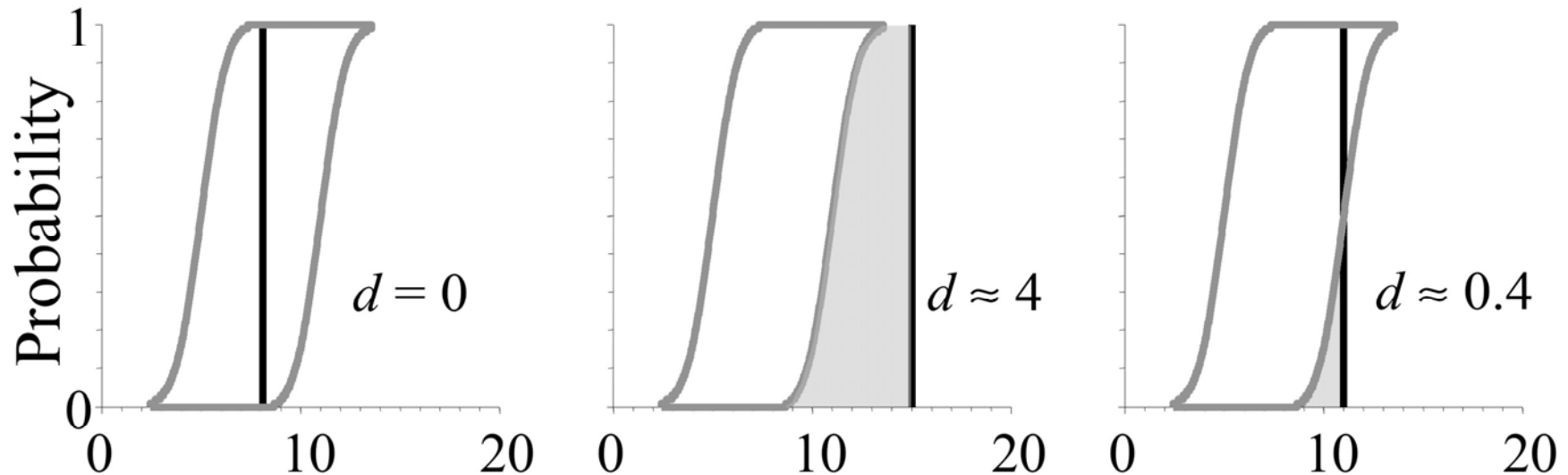


Mapping of Epistemic Uncertainty from an SRQ to a Probability





Validation Metric for Aleatory and Epistemic Uncertainty in the Simulation



- When epistemic uncertainty exist in the simulation, or in the measurements, the validation metric can be **zero**
- This does **not** mean perfect agreement
- It means there is **no evidence** that the simulation and experiment are in disagreement



Generalizing the Validation Metric for Aleatory and Epistemic Uncertainty

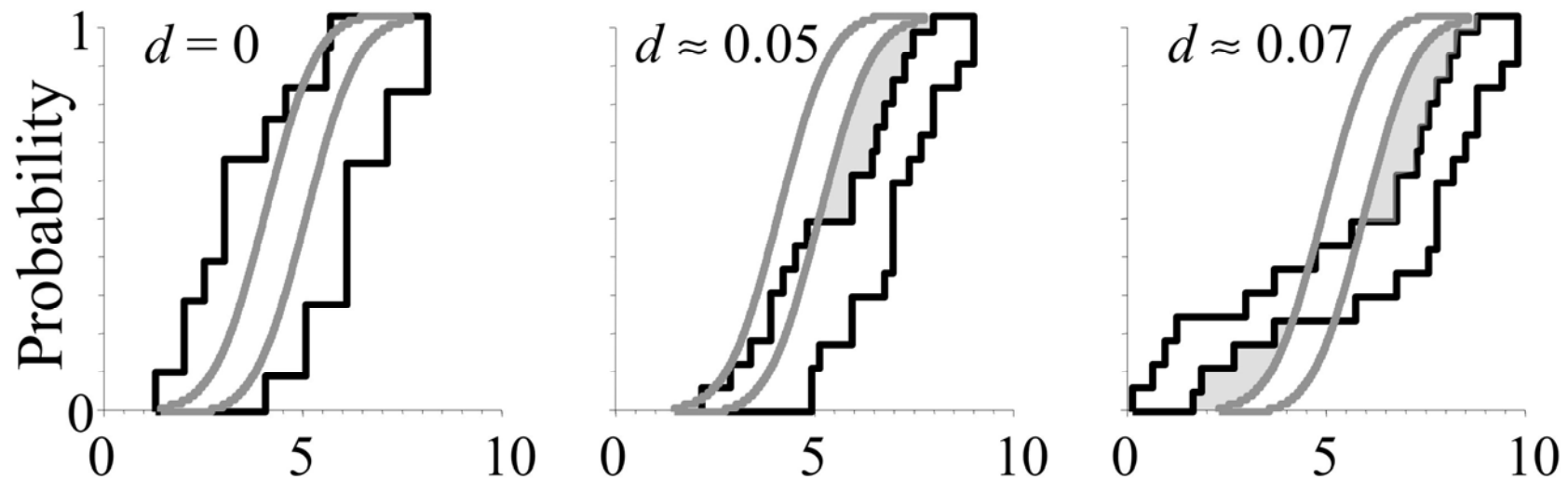
- The validation metric is now defined as

$$\int_{-\infty}^{\infty} \Delta([F_R(x), F_L(x)], [S_{nR}(x), S_{nL}(x)]) dx$$

- where subscripts L and R denote the left and right bounds for any epistemically uncertain CDFs
 - and $\Delta(A, B) = \min_{\substack{a \in A \\ b \in B}} |a - b|$
- This metric is **no longer** a true mathematical metric because the measure can attain zero without simulation and experiment being identical

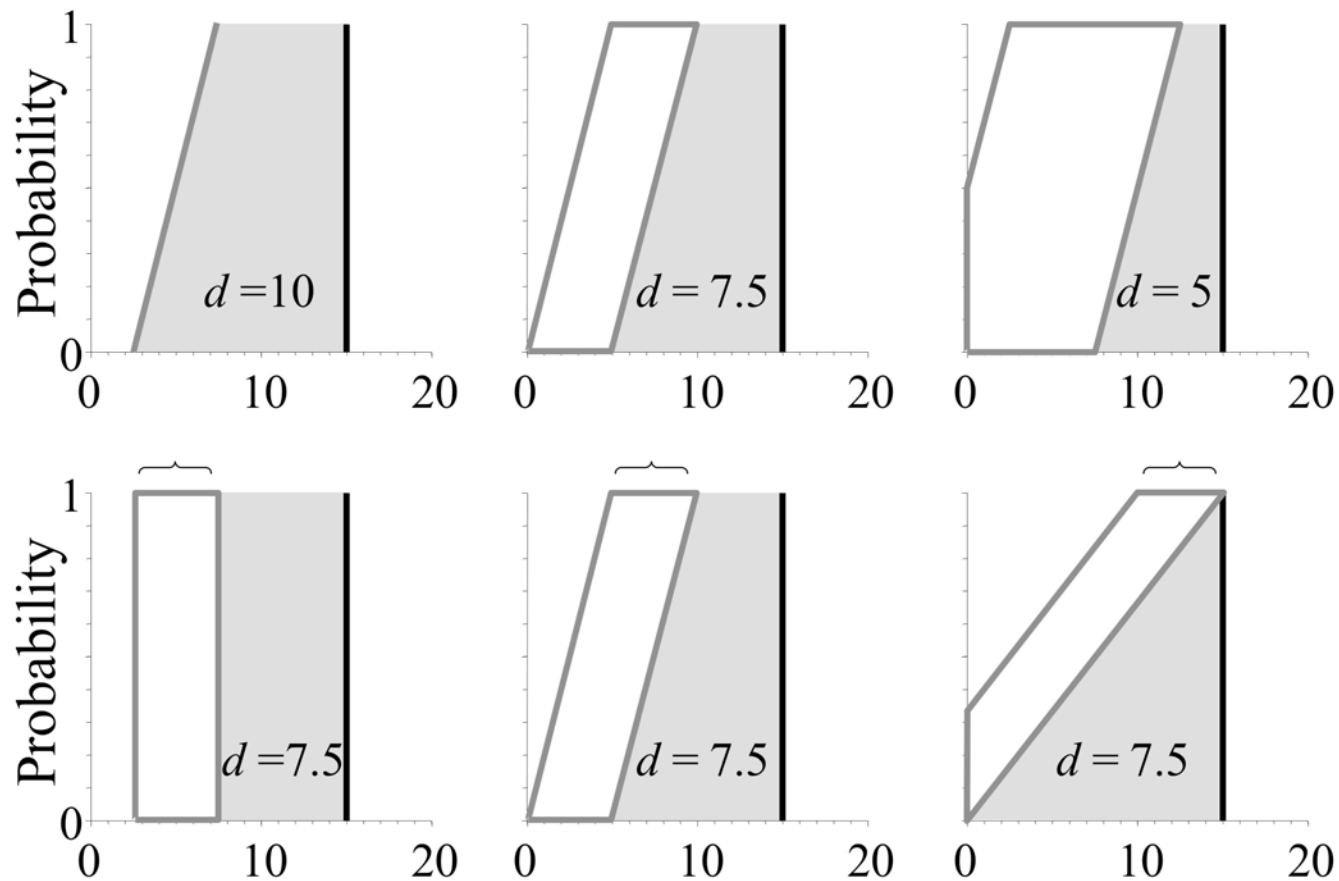


Validation Metric for Aleatory and Epistemic Uncertainty in both the Simulation and Experiment



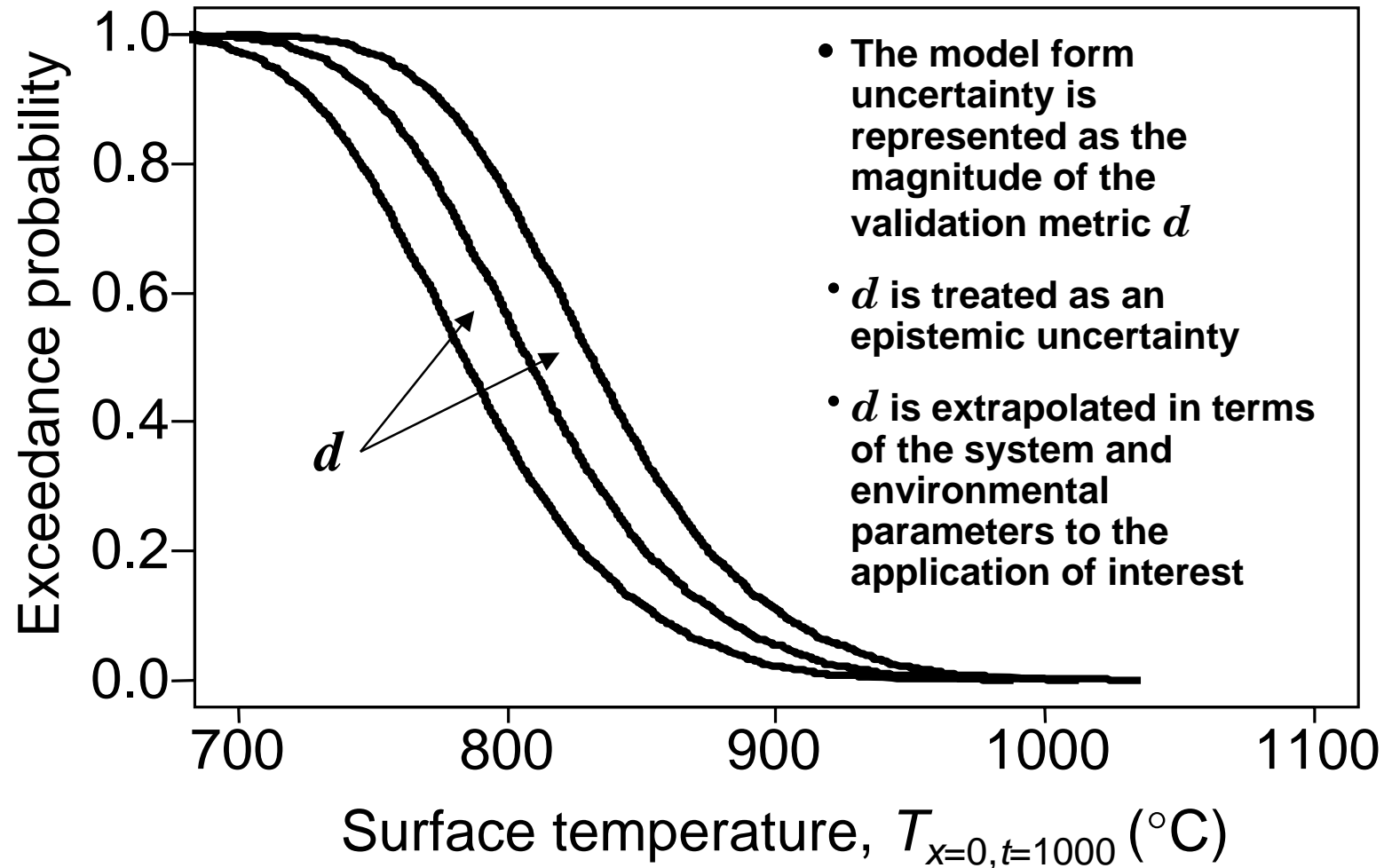


Example of Increasing Epistemic and Aleatory Uncertainty in the Simulation





How is the Validation Metric Result d Used in a Prediction?





Concluding Remarks

- We believe it is essential to explicitly quantify the mismatch of our models in comparisons with experimental data
- Epistemic uncertainty should be characterized using intervals, then use either:
 - Second order probability
 - Dempster-Shafer theory
 - Probability boxes

to propagate uncertainty from inputs to SRQs

- Improve methods are needed to extrapolate the validation metric, d , to the application of interest
- We must continue to find ways of testing our predictive capability by “blind” comparisons with experiments

**Goal: Improved Risk-Informed Decision Making
For Engineering Systems**