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Introduction to the Real-Space Model Validation Approach and Its Advantages vs. the ASME VV10 and VV20 Validation Approaches*

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The Significance of Aleatory vs. Epistemic uncertainty in model validation

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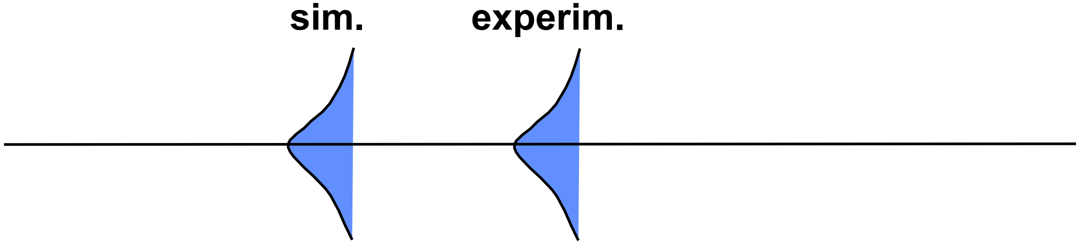
These PDFs line up perfectly. Is the model prediction perfect or likely biased?



- **Answer: it depends pivotally on the nature of the uncertainty represented by the PDFs**
  - Perfect model if the PDFs represent populations of results from a stochastic system tested multiple times w/ no other uncertainty in the tests (aleatory uncertainty only)
  - Model likely has error if the PDFs represent only epistemic uncertainty (lack of knowledge) regarding the deterministic value of a response

Treatment of Aleatory and Epistemic Uncertainties in Model Validation

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- **Real Space approach can be viewed as an <u>extended hybrid</u> of other well-established validation frameworks:**
  - **ASME V&V20 2009 *Standard for V&V in CFD and Heat Transfer***
    - Subtractive-difference metric is geared for validation of models of effectively deterministic systems (i.e., no "traveling" uncertainties intrinsic to the model)
    - Full treatment of epistemic lack-of-knowledge type uncertainties in model discretization solution error and modeled experimental ICs/BCs and measured experimental inputs and outputs
    - 2-parameter probabilistic uncertainty treatment based on mean and stdev.
  - **ASME V&V10.1 2012 *Supplement for V&V in Computational Solid Mech.***
    - built for validation of models of stochastic systems with significant aleatory variability
    - uses Ferson/Oberkampf "Area" validation metric for mis-match of sim. & exper. CDFs
    - can be extended to treatment of aleatory <u>and</u> epistemic uncertainties (e.g., with a segregated "Probability box" uncertainty representation per Ferson & Oberkampf)
    - ignores some important types of experimental epistemic uncertainty that ASME VV20 and Real Space include
  - **Real Space: no restrictions, + significant extensions**

Concept of “Traveling” and “Non-Traveling” Uncertainties

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Traveling Uncertainties **are intrinsic to the model being validated**

They come with the model as a consequence of model-form error and/or lack of knowledge about values of parameters in the model.

They are consistent between the validation conditions and model applications beyond the validation activity.

Non-Traveling **uncertainties are particular to the validation activity**

They are outside the traveling model of extrapolation interest

- **e.g., experimental measurement uncertainties and model discretization related solution uncertainty in the validation activity**

Real Space vs. Subtractive-Difference Transform Representation of Model Discrepancy

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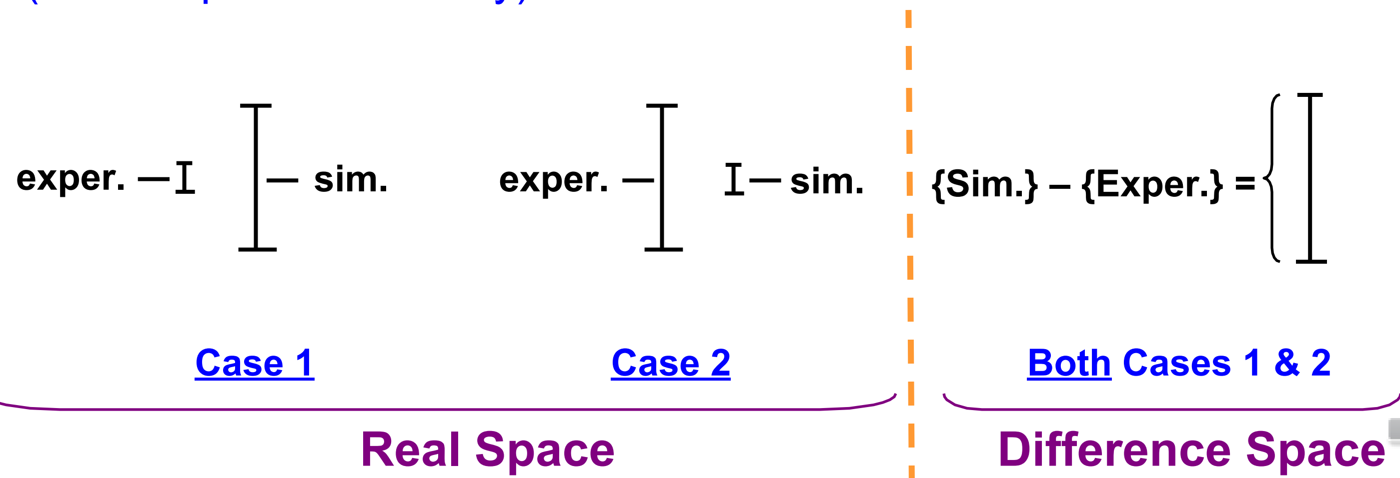
- Subtractive difference is a popular way of comparing data against model predictions for model validation assessments (but best used for only non-traveling epistemic uncertainties)
- The subtractive difference transform yields a <u>less definitive</u> validation result vs. staying in real space – see example below
- Subtractive Difference has non-unique mapping from real space to transform space, as do other (<u>perhaps all</u>?) validation metric discrepancy transforms
- Subtractive Difference non-uniqueness is not a problem if constrained to <u>Non-Traveling</u> epistemic uncertainties, but is a problem for <u>Traveling</u> epistemic uncertainties (to be explained verbally)

<u>Example</u>
with Traveling Epistemic uncertainties in the model and differing risk connotations with its use



ASME VV10 Applicability to One Experiment with Epistemic Uncertainty Only

- **Depending on the details, ASME VV10 <u>does in some cases</u> properly account for <u>traveling and non-traveling</u> epistemic uncertainties in the model**
- **But does not show how to handle complex experimental uncertainty:**
  - random and systematic components of error and correlated errors in measurements of inputs and outputs
- **ASME VV20 has demonstrated complex experimental uncertainty with <u>probabilistic non-traveling</u> uncertainties**
- **Real Space has demonstrated complex experimental uncertainty with <u>probabilistic and/or interval</u> <u>traveling and/or non-traveling</u> uncertainties**

Model Builder's Risk vs. Model User's Risk
with respect to systematic uncertainty in experiment conditions

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- Where place burden of proof?
  - *Optimistic* stance: Assume model is unbiased if don't have positive proof that it is biased (outside expr. uncer.)
    - Oberkampf & Roy: "*When the simulation is a P-Box due to insufficient information provided by the validation experiment, the model is given more leeway in comparing with the experiment, as is appropriate*."
    - "Free lunch"— the more experimental uncertainty, the more model-bias leeway allowed
    - eliminates Model Bldr.'s risk but increases Model User risk
  - *Conservative*: Treat model as potentially biased up to magnitude allowed by resolution uncertainty in expers.
    - Real Space – reduces Model User's risk but increases Model Builder's risk
    - ASME V&V20 – similar

<u>Now Consider Multiple Replicate Tests with Stochastically Varying Systems</u>

- For validation of models with traveling aleatory uncertainty that represents the stochastic variability in the systems
- random/aleatory variation of the systems from test-to-test
- test-to-test random/aleatory variation of measurement errors on inputs and/or outputs ("random" uncertainties)
- test-to-test effectively constant errors in measurements of inputs and/or outputs ("systematic" uncertainties)

Real Space comparison for Stochastic Experimental and Simulation Results

(at same input conditions, shown side-by-side for comparison)

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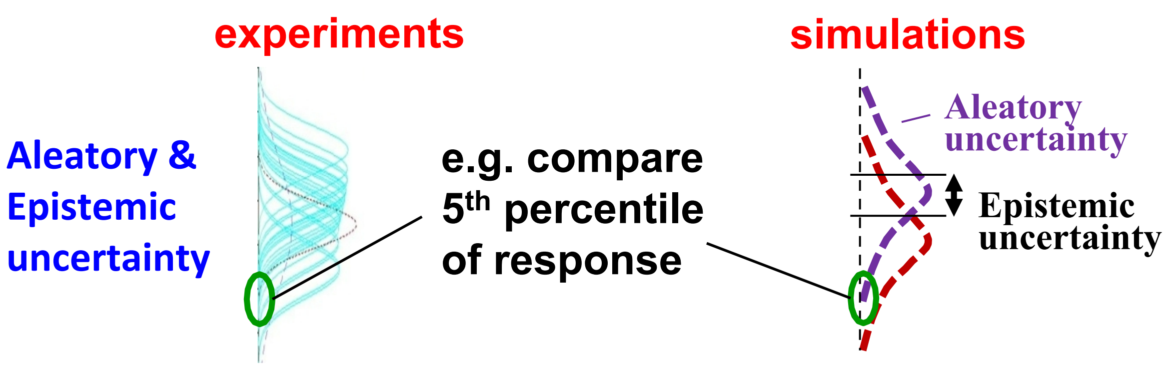
- **Compare statistical measures of response, not whole CDFs**
- **Use sparse-sample UQ methods to bound experim. and sim. statistics**



- **Intuitive visual indication of how accurate the model is, on several fronts:**
  - **Means** of the predicted and experimental populations
  - **Variances**
  - **Percentiles**
  - **Range of response %, e.g. the "central" 95% between 2.5 and 97.5 percentiles**

  (These last two account for combined uncertainty in mean, variance, and possible higher moments of stochastic response and are found to be the most useful in practice)

- **Percentile comparisons are particularly useful for validation of models to be used for analysis of performance and safety margins**

VV20 Subtractive-Difference Metric prevents proper handling of Modeled Variability among a Population of Stochastic Systems in Replicate Experiments

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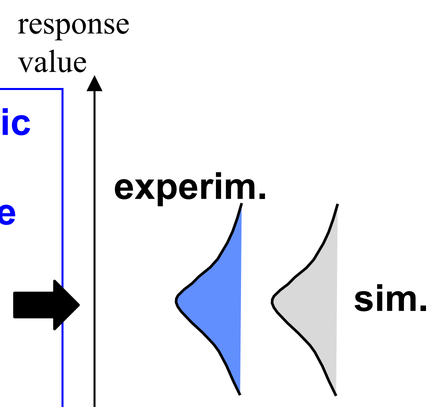
Let simulated stochastic variability from the model exactly equal the variability of many real systems tested

- Traveling stochastic variability



- **Conditions**: no measurement errors in the experiments; and large # of tests
- Observed response variability is due to unit-to-unit stochastic variability of the tested systems, and not due to testing variability

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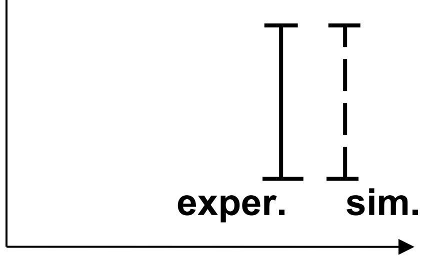
Real Space approach

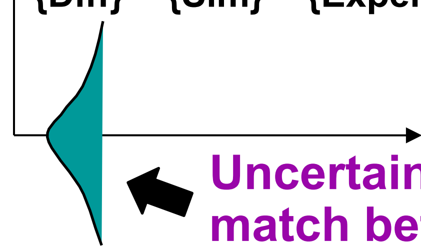
✓ works; no model error indicated



ASME VV20 Sub-tractive Diff. Metric

- non-zero uncertainty results--attributed as possible model bias

{Diff} = {Sim} – {Exper}



Uncertainty should be zero for exact match between experim. and sim. results

VV10 Area Metric

✓ works; no model error indicated

- zero area between exper. and sim. CDFs

Non-Uniqueness of Area Metric of CDF Mismatch

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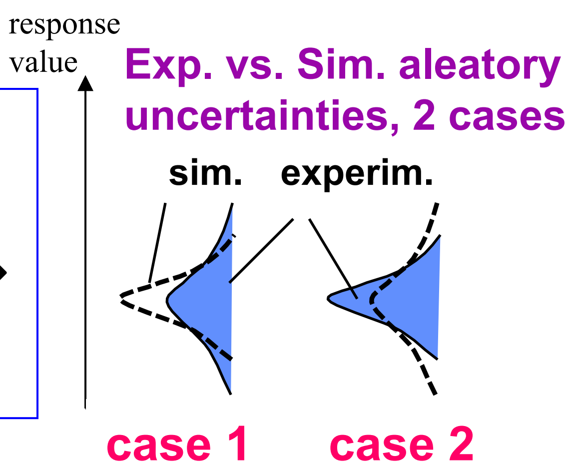
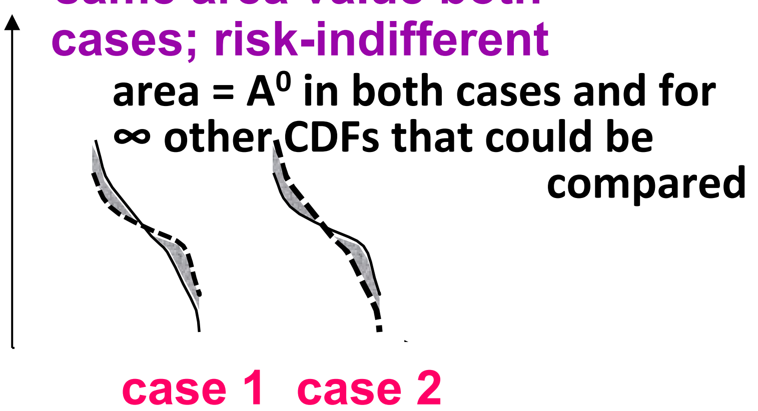
Consider two cases where relative uncertainties in experiment and simulation results are very different



Area Metric

- same area value both cases; risk-indifferent



- non-uniqueness of Area Metric can hide prediction risk and undermine metric use for extrapolation (next slide)

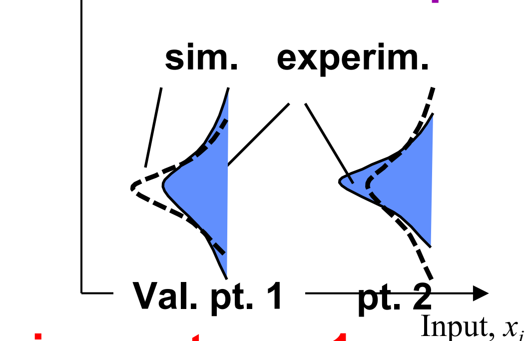
Real Space method

- like-percentiles of CDFs are compared
- Unique and more granular quantification of how CDFs differ
- reveals different prediction risks in these two cases

Area Metric Non-Uniqueness can also obscure the Trend of Model Error

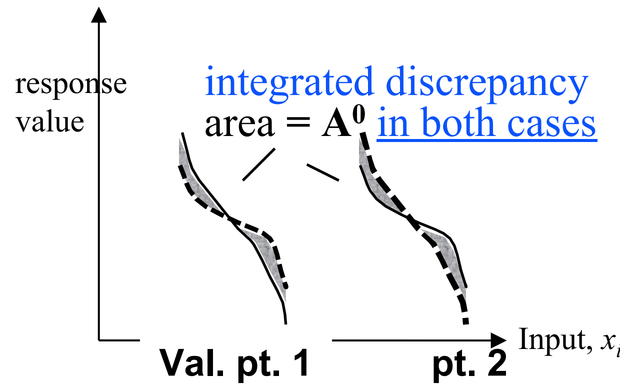
Real Space method

- reveals differing sim. & exper. trends



Area Metric

- same areas for diff. model trend errors



circumstance 1

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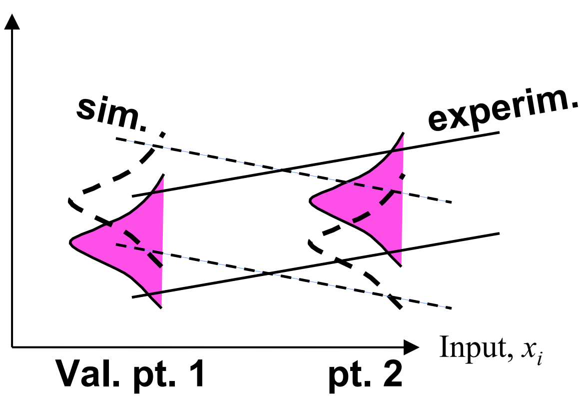
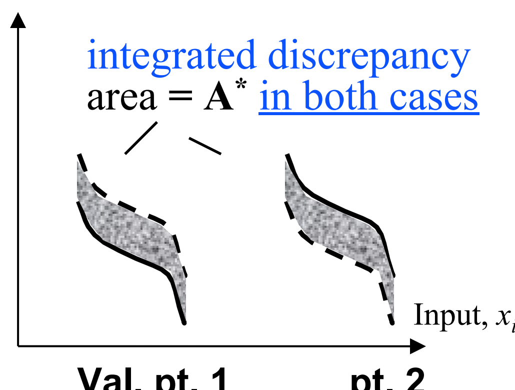
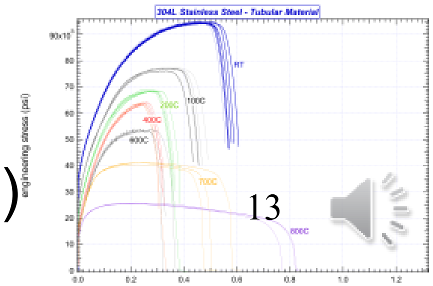
circumstance 2





Other Differentiating Features of the Real Space methodology

- **Explicitly accounts for epistemic uncertainty arising from small sample sizes (limited numbers of replicate tests) in experimental characterization of mtls., systems**
  - a dominant or significant uncertainty in many cases
- **The RS framework has demonstrated protocols for treatment of the following representations of uncertainty, individually and in combination:**
  - **Interval**
  - **Distributional (probability density functions)**
  - **Discrete (non-parametric)**
    - e.g. different turbulence model forms and discrete stress-strain curves (functional data)

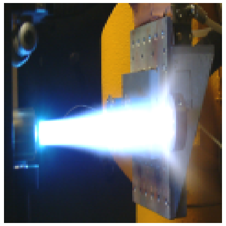
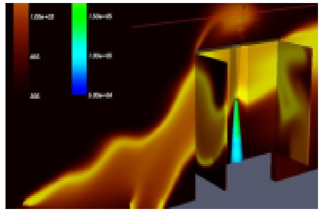


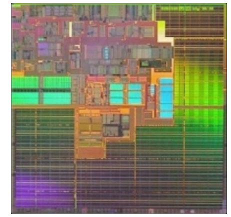
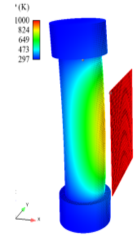
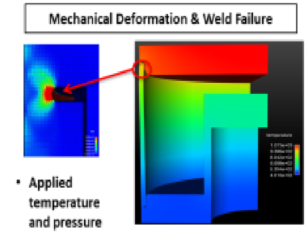
Support for Prediction Bias Correction and Extrapolation

- **ASME VV10**
  - A possible extension exists per Roy & Oberkampf, but only when the experimental and simulation PDFs don't overlap significantly.
    - Then the Area metric has a physical connotation of the difference between the means of the distributions, so a mean correction can be applied to the simulation PDF (but not percentile-by-percentile like the Real Space method allows).

- **ASME VV20**
  - no established connectivity to bias-correction or extrapolation

- **Real Space**
  - Prediction bias correction for a selected percentile of response and Predictor-Corrector extrapolation of the correction, with extrapolation UQ scaled to extrapolation distance

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- **The Real Space validation methodology is versatile and practical, geared for:**
  - expensive computational models (minimal # of simulations)
  - stochastic phenomena and models
  - multiple replicate experiments with <u>random</u> and <u>systematic</u> uncertainties on experimental inputs and outputs
  - few replicates (sparse data)
  - rollup of various types, sources, and representations of uncertainty
    - aleatory and epistemic
    - traveling, non-traveling
    - probabilistic, interval, and discrete variables and functions

- **Real Space Validation results are:**
  - relatively straightforward to interpret for model adequacy and bias corr.
  - especially relevant for assessing models to be used for the analysis of performance and safety margins