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The Real-Space Model Validation Approach as a Unifying? Extended Hybrid of the ASME VV10 and VV20 Approaches

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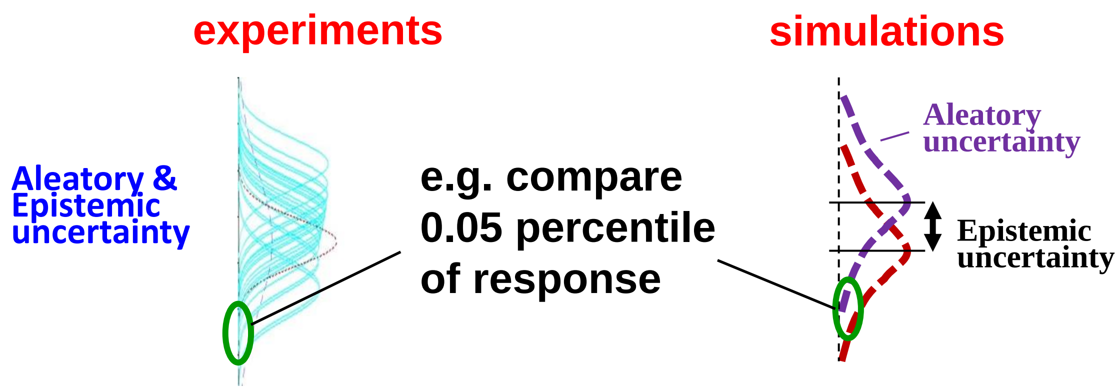
Real-Space Uncertainty Accounting and Comparison System for Experimental and Simulation Results —applicable in both calibration and validation



- **General problem involves <u>Probability Boxes</u> of experimental and sim. uncer.**
- **Intuitive visual indication of how accurate the model is, on several fronts:**
  - **<u>Means</u>** of the predicted and experimental populations
  - **<u>Variance</u>** of the predicted and experimental populations
  - **<u>Percentiles</u>** of the predicted and experimental populations

<u>granular quantification</u> of how the model is doing, as compared to validation metrics of integrated measure of mismatch at whole-distribution level

- **Percentile comparisons are particularly useful for calibration and validation of models to be used for analysis of performance and safety <u>margins</u> (e.g. QMU).**

5 Levels of Increasing Rigor in Treatment of Experimental and Simulation Uncertainties in Model Validation

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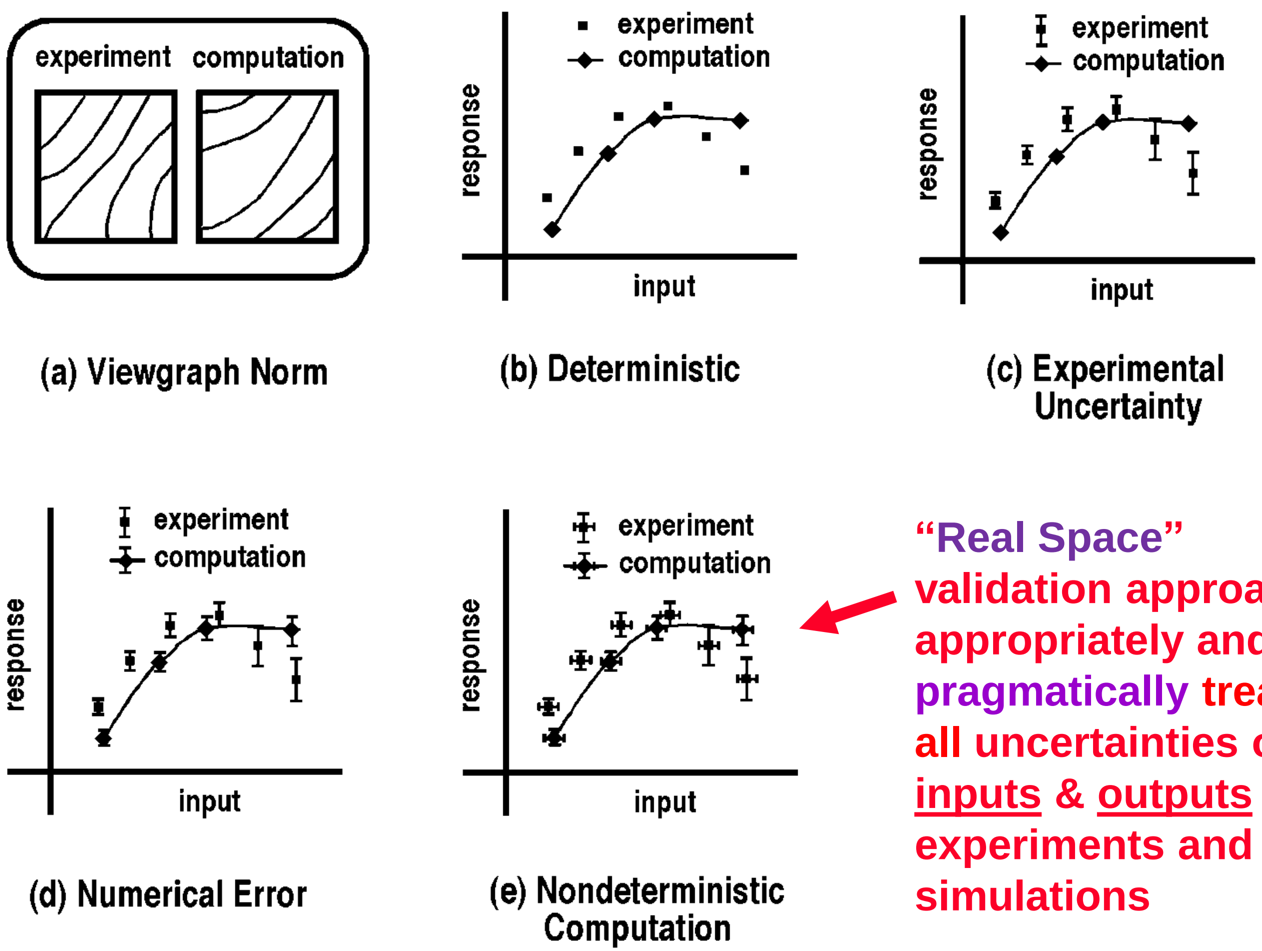

"Real Space" validation approach appropriately and pragmatically treats all uncertainties on <u>inputs</u> & <u>outputs</u> of experiments and simulations

Figs from "Increasing Quality of Validation Metrics," Sandia National Laboratories report SAND2003-3769, Oberkampf, Trucano, & Hirsch

Consider Subtractive Difference of <u>Deterministic</u> Experimental and Model Results as Fcn. of Input *X*

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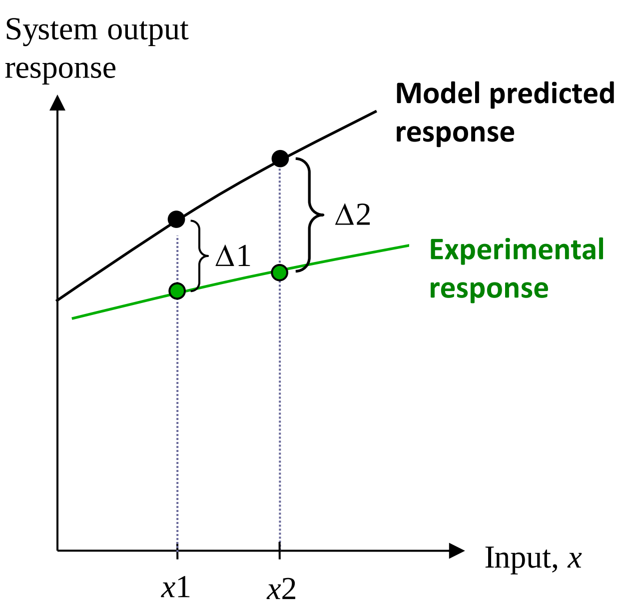
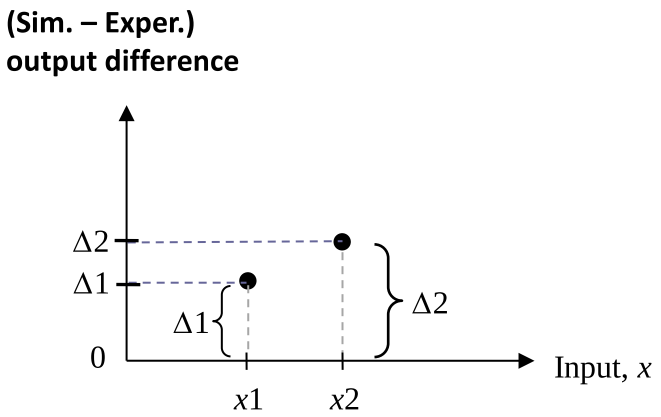
Simulated and Experimental results at various input values of *x*.



<u>Subtractive Differences</u> of results



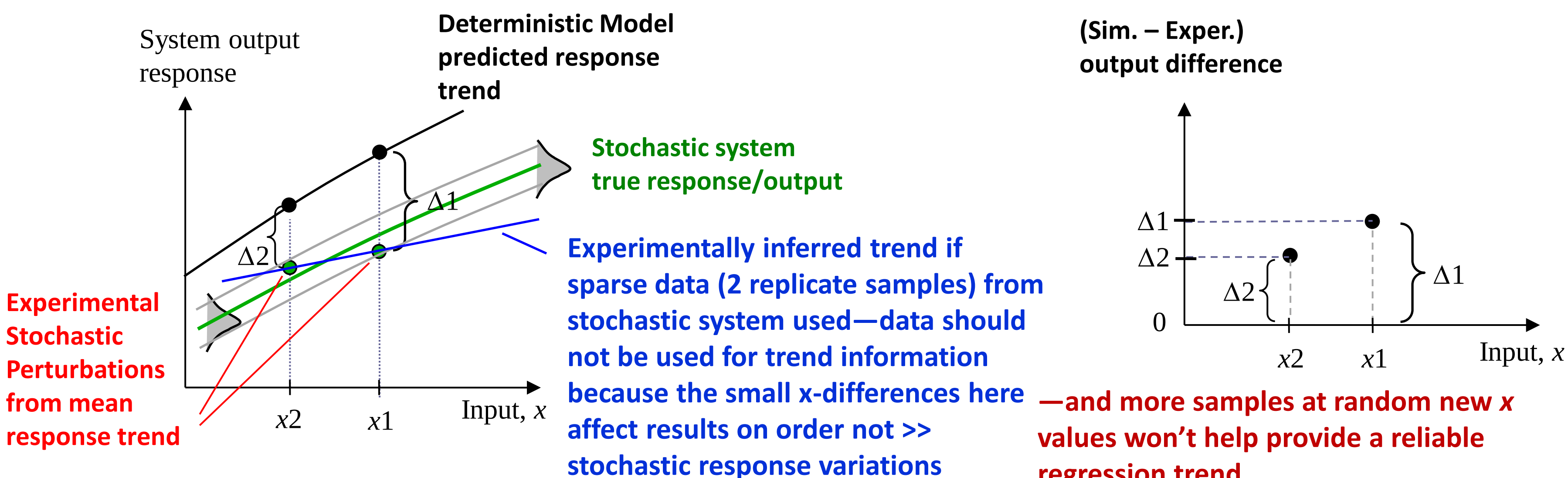
For now <u>assume</u>:

- **No measurement errors on inputs or outputs**
- **Negligible solution error/uncertainty in model predictions**

Change Context to
Stochastic Systems and Replicate Experiments

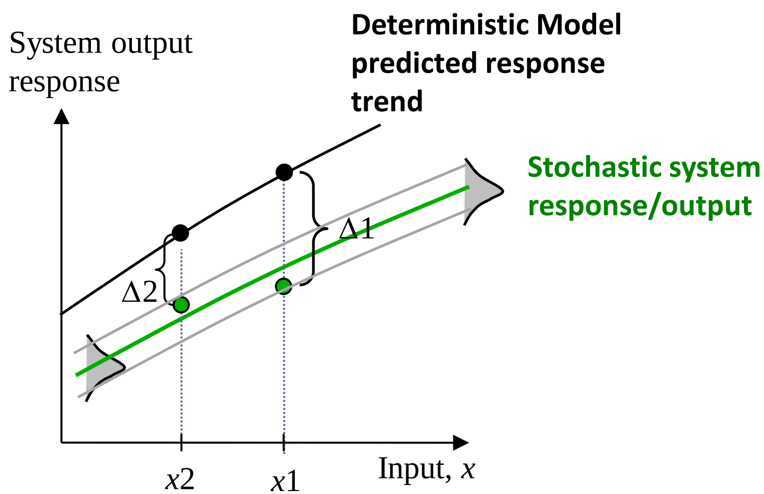
⇨ Aleatory Experimental Uncertainty (Variability)

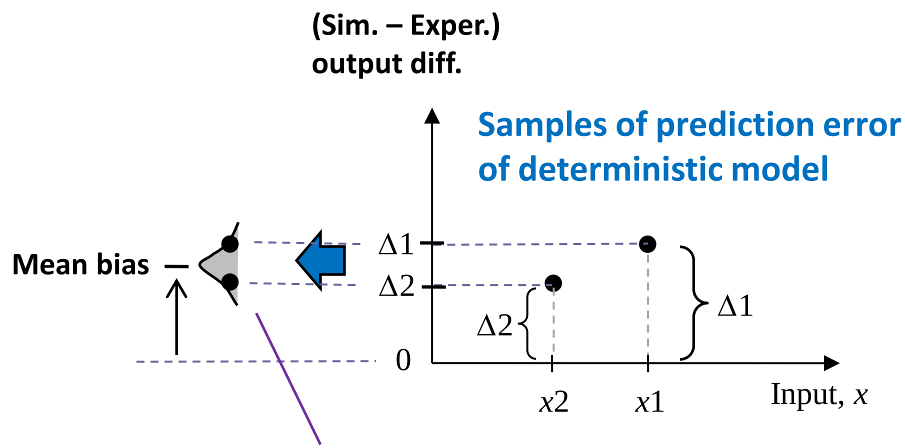
- Complex engineered systems usually involve non-trivial geometric and physical behavior variability, ("stochastic" systems).
- Replicate experiments can illuminate the effects of stoch. system variability by examining output/response variability in repeated tests at the ~same input conditions.
- Input conditions often cannot be exactly repeated in replicate tests, but instead are controlled to within small changes.
- E.g, in the following we try to control the input condition to a value *x*_target, but in two tests we obtain slightly different values *x*1 and *x*2; *x*1 ≈ *x*2 ≈ *x*_target



Stochastic Systems and Replicate Experiments — Aleatory Experimental Uncertainty

- Nonetheless, the model results and experimental data can be used to characterize mis-prediction of the deterministic model vs. experimental stochastic system response.

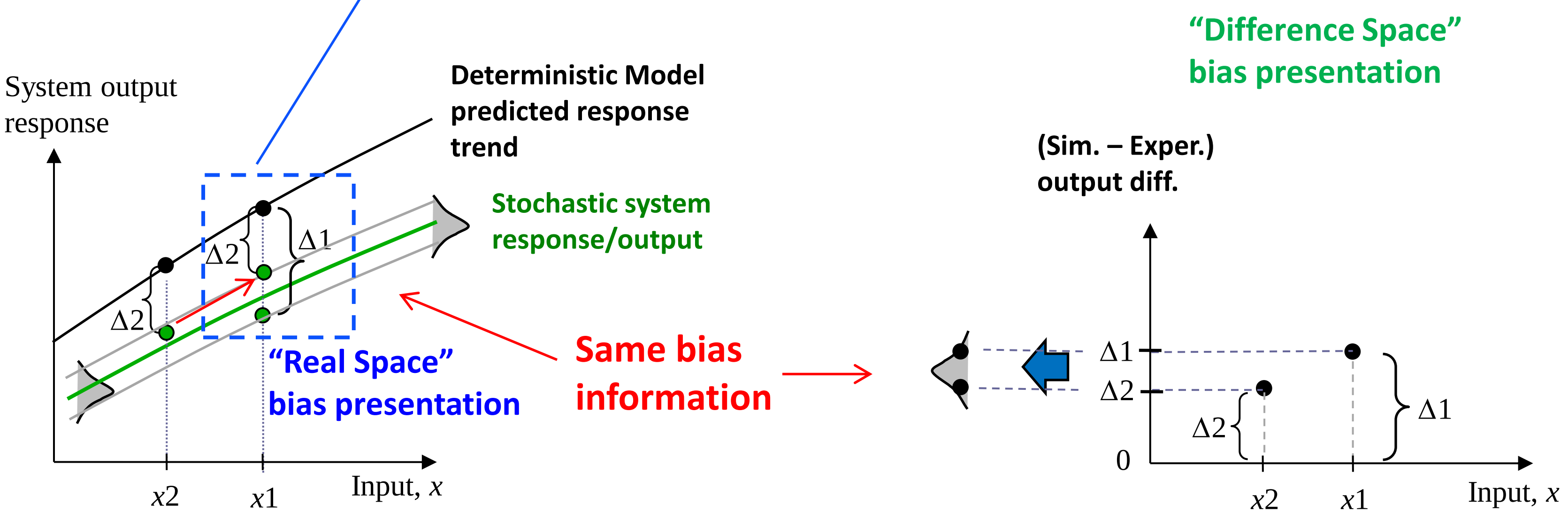




Distribution of Differences:
samples of prediction error can be said to come from a parent population (PDF) of model prediction bias at the ~target input conditions
***x*_target ≈ *x*1 ≈ *x*2**
in the validation assessment.

Stochastic Systems and Replicate Experiments — Aleatory Experimental Uncertainty

- **Thus, one can consider the samples of prediction bias, $\Delta 1$ and $\Delta 2$, to be from the ~same PDF of prediction bias at input values *x* in the vicinity of *x*_target ≈ *x*1 ≈ *x*2**
- **Can go further and pick a convenient *x* value to consolidate the prediction bias information, realizations $\Delta 1$ and $\Delta 2$, for any further validation or calibration analysis**
- **E.g., choose input level *x*1 and consolidate prediction-bias information there in order to carry out any further val. or cal. analysis**



Advantage of Real Space Consolidation of Replicate Results to Single Input Value

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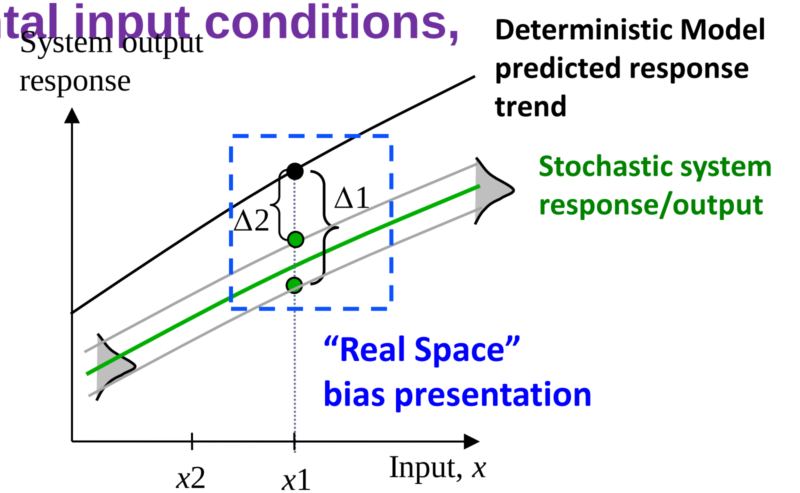
Calibration

- allows calibration of model at one set of input conditions instead of many perturbed sets, while addressing the same full set of bias information
- calibrations traditionally formulated in terms of cal. params. iterated so real-space response values are matched, not cal. parameter deltas calibrated to match output response deltas

Validation

- allows propagation of model input uncertainties and val. assessment for one set of experimental input conditions, instead of multiple perturbations



Consolidated Bias Presentation originally arrived at from different perspective: <u>Real Space Validat'n</u>.

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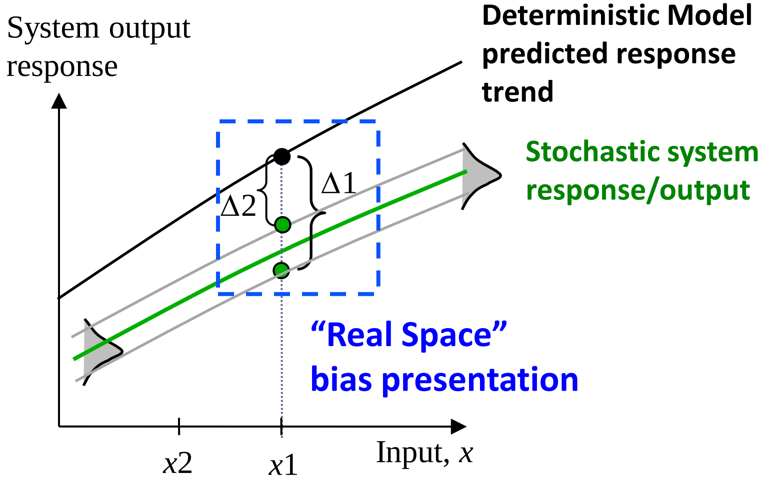
- **The development to this point reconciles the <u>Difference Approach</u> with prior results arrived at from a different perspective—the <u>Real Space model validation approach</u>.**
- **RS model validation methodology arrives at <u>completely consistent</u> results, but from a different direction and w/ a <u>different interpretation</u>**
  - **use the model to "normalize" or <u>*consolidate*</u> replicate data to the same reference input condition**
  - **The consolidated data (green dots) are viewed as sample realizations of response variability in the replicate tests of the stochastic system**



- **<u>Duality Relationship</u>: consolidated samples of prediction bias, Δ1 and Δ2 at *x*1, are consistent with the RS view that the green dots are <u>samples of the stochastic response</u> at *x*1**

ASME VV10 Supplement's <u>Starting Point</u> for Response Samples of Stochastic Systems

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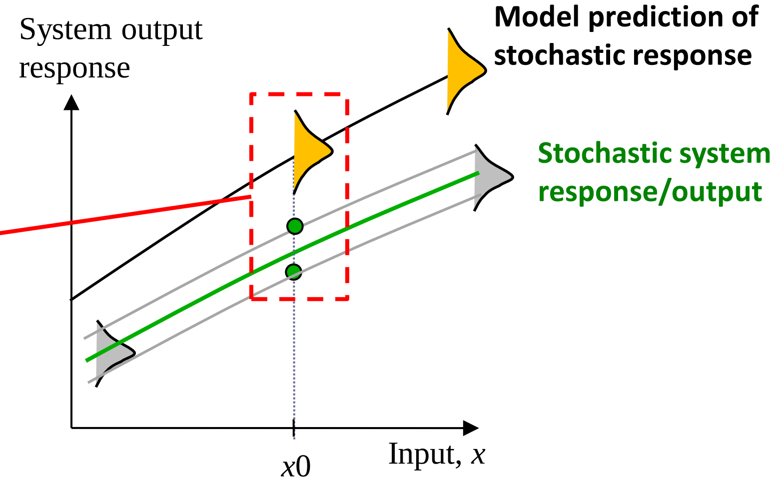
- VV10 starts from a condition of <u>consolidated response samples</u> when stochastic systems and replicate tests are involved
- Doesn't show how to deal with experimental inputs that cannot be exactly repeated in replicate tests —the reality in many/most val. & cal. experiments.
- Having shown how to transform to the starting point for VV10, we go on to compare from this starting point



- <u>**VV10 Area Metric**</u>
  - **CDF of replicate experimental results is formed, as is a CDF of predicted stochastic response**

  - **<u>area</u> between simulated and experimental CDFs is a measure of mismatch between sim. and exper. stochastic response**

Handling Sparse Experimental Data

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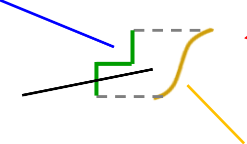
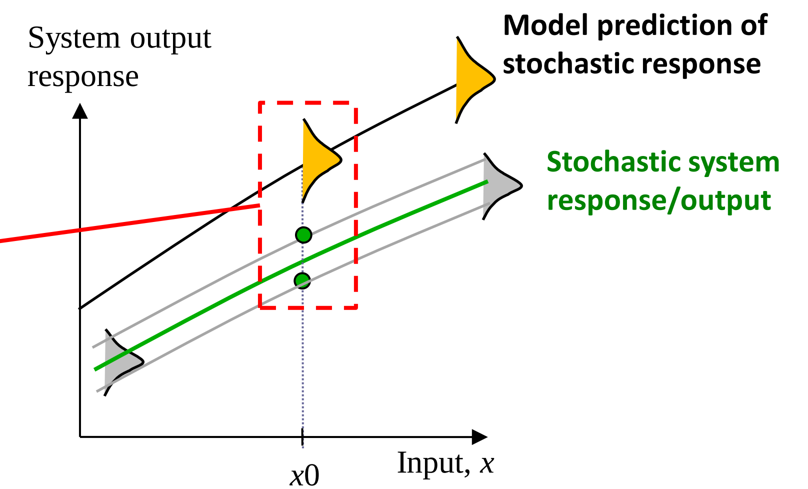
- **VV10 does not present an approach for dealing with the <u>large</u> epistemic uncertainty in CDFs built from few samples.**
- **Real Space method does, see ASME V&V 2015 Symposium presentation "Approximate Probability Boxes and Other Shortcuts…," V. Romero.**

- **Sparse-Data CDFs are not "anchored" in any way**
- **Adding more data not only adds more stair-steps to the CDF, but also <u>shifts</u> the CDF and alters it's variance**



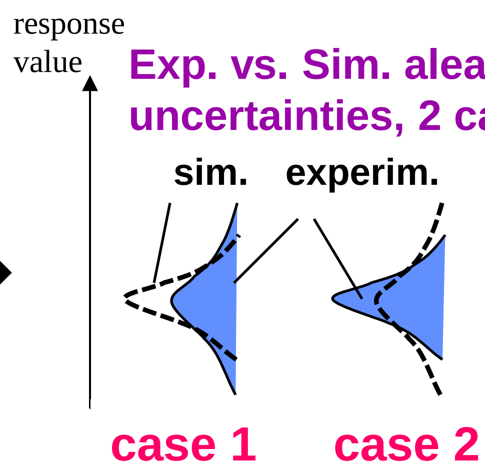
- **Highly uncertain val. metric value from sparse data is not accounted for in VV10 approach.**



Non-Uniqueness of Area Metric of CDF Mismatch

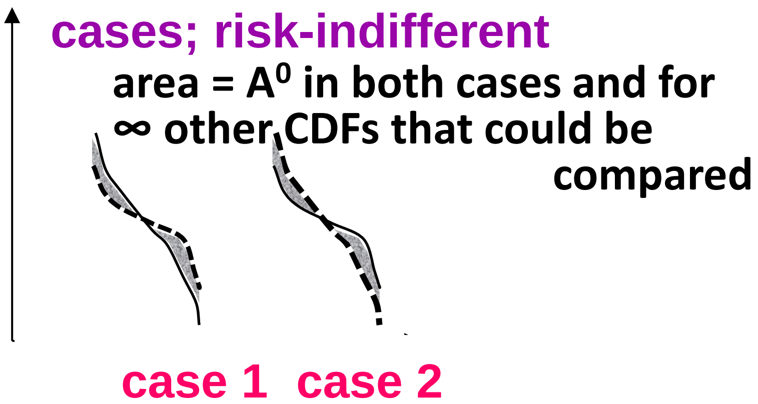
Consider two cases where relative uncertainties in experiment and simulation results are very different

Exp. vs. Sim. aleatory uncertainties, 2 cases



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)

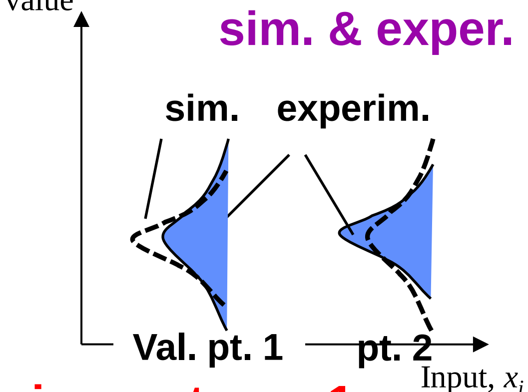
Real Space method

- 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

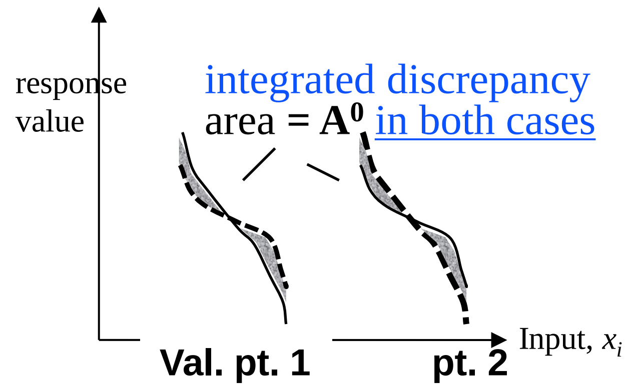
Real Space method

- reveals differing sim. & exper. trends



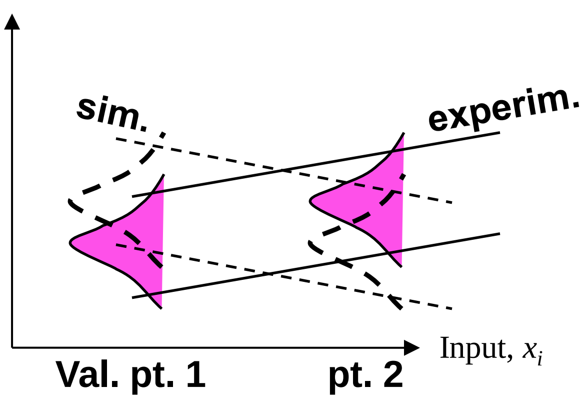
Area Metric

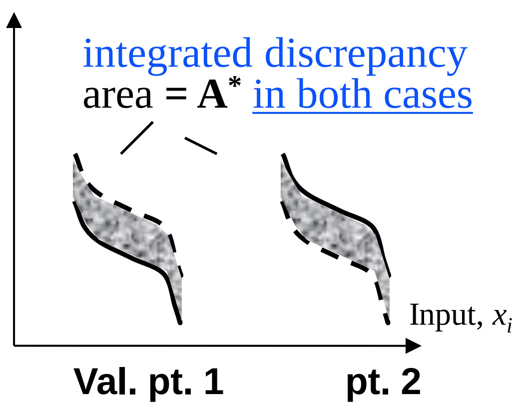
- same areas for diff. model trend errors



circumstance 1

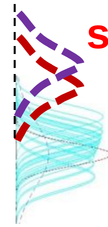
circumstance 2





Handling <u>Epistemic</u> Uncertainty

- **Validation and Calibration often involve significant aleatory <u>and</u> epistemic uncertainties in the experiments and simulations.**
  - ⇨ epistemically uncertain CDFs of the aleatory variability in the experiments and predictions



• **VV10 does not present an approach for dealing with epistemically uncertain experimental and/or predicted CDFs, but <u>"Probability Box" extensions</u> exist in the literature for doing so (e.g. Oberkampf, Ferson, Roy)**

• **These extensions do <u>not</u> appropriately handle "<u>traveling</u>" epistemic uncertainties that are an intrinsic part of the model being validated, e.g. uncertainty parameterized into the model to account for model-form error**

***Traveling* – model quantities and uncertainties proposed to "travel" consist-ently from the validation space to intended application space. These define the (traveling) 'model' in model validation.**

***Non-Traveling* – quantities and uncertainties that are exclusive to the validation space. These are <u>outside</u> the control volume or boundary that contains and defines the traveling model.**

Handling <u>Epistemic</u> Uncertainty

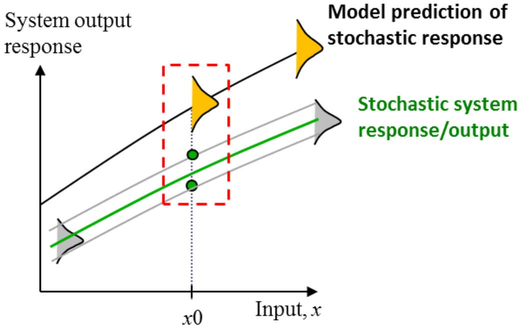
ASME VV20 Standard for V&V in Computational Fluid Dynamics and Heat Transfer

- **treats <u>non-traveling</u> epistemic uncertainties appropriately**
- **does not appropriately treat <u>*traveling*</u> epistemic uncertainties**

- **VV20 and Real Space approaches for handling epistemic uncertainties are <u>procedurally different</u>**
- **But the results can be shown to be <u>equivalent</u> for the <u>non-traveling</u> subset of epistemic uncertainties**
- **<u>Different but Equivalent</u>:**
  - analogous to the <u>duality</u> relationship presented earlier between variance of prediction bias *vs.* experimental variance

VV20 Uncertainty Treatment improperly treats Model Predictions of Stochastic Response (Traveling Aleatory Uncertainty in the Model)

- **VV20's Subtractive Difference operation does not appropriately extend to model predictions of stochastic response —see example on next slide**



- **VV20 may have to move to Probability Boxes or other uncertainty representation and accounting approach to appropriately handle validation involving stochastic systems and models.**

- **Furthermore, neither VV20 nor VV10 currently explicitly account for randomly varying measurement errors in multiple replicate experiments. Real Space does.**
  - **Especially important when only a few replicates are involved.**

VV20 Uncertainty Treatment is Improper when Model Predictions of Stochastic Aleatory Uncertainty are involved

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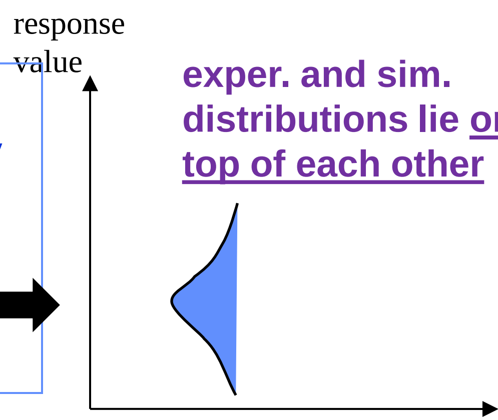
E.g., let simulated stochastic variability of system exactly equal variability of real system tested many times



exper. and sim. distributions lie <u>on top of each other</u>

- <u>Conditions</u>: 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

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Real Space approach

✓ works; no model error indicated when like percentiles compared

ASME V&V20 Sub-tractive Diff. approach

- attributes uncertainty as model bias

{Diff} = {Sim} – {Exper}

PDF should have zero width for exact experim. / sim. variability match above

VV 10 Area Metric

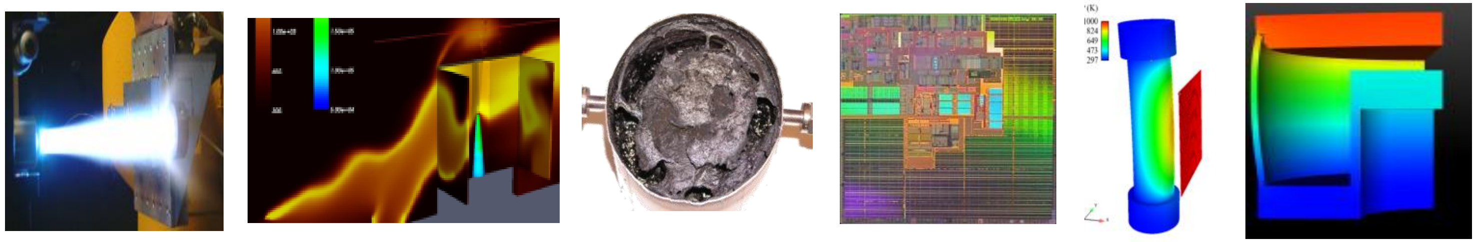
✓ works; no model error indicated

Real Space approach can be viewed as an <u>extended hybrid</u> of published ASME frameworks

—contains and extends beyond their capabilities

– **ASME V&V20 2009 *Standard for V&V in CFD and Heat Transfer***
  - geared for validation of deterministic (non-stochastic) systems
  - no aleatory-epistemic differentiation
  - equivalent to Real Space for probabilistic uncertainty and non-traveling epistemic uncertainty

– **ASME V&V10 2012 *Supplement for V&V in Computational Solid Mechanics***
  - built for validation of stochastic systems
  - segregates aleatory and epistemic uncertainties (Prob. boxes)
  - uses Ferson & Oberkampf "area" validation metric (CDF matching)
  - does not show how to incorporate important types of experimental epistemic uncertainty that ASME VV20 and Real Space do



- **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 random and systematic uncers.
  - few replicates (sparse data)
  - rollup of various types, sources, and representations of uncertainty
    - aleatory and epistemic
    - probabilistic, interval, and discrete variables and functions

- **Real Space Validation results are:**
  - relatively straightforward to interpret
  - especially relevant for assessing models/quantities to be used in the analysis of performance and safety margins (QMU)

Closing

The Real Space validation approach will be featured in Joint Army/Navy/NASA/Air Force (JANNAF) document:

"*Advances in Model V&V, UQ, and Simulation Credibility for Propulsion and Energetics*"

due out in Sept. 2015.