

Sub-Grid Closure Validation: Burden of Extracting Model Form Discrepancy

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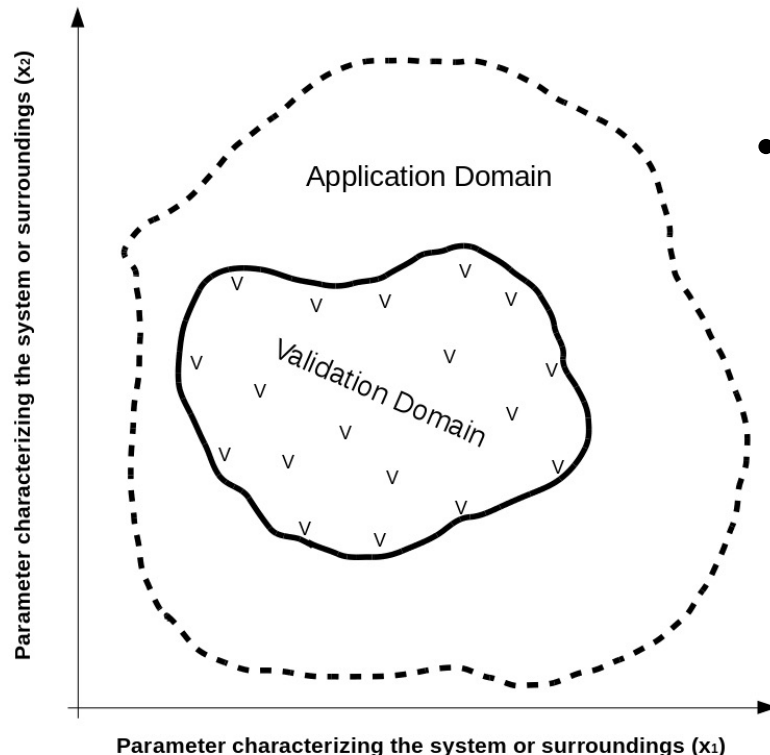


Assessing the Credibility of CFD Results



- **Computer simulations are playing an ever-increasing role in the design and development of combustor systems.**
 - Culture has morphed from one that historically relied solely on ground testing to one that is increasingly more reliant on computational simulation.
 - Justification for this increased reliance hinges on:
 - a) improvements in verification practices
 - b) a quantitative understanding of the physics available in the modeling (i.e., validation)
 - c) the ability to perform a comprehensive uncertainty assessment of simulation results
 - **Inadequate validation data is a key limiting factor** preventing CFD from playing a larger role in the engineering design and development of combustion systems due to the presence of additional complex physical phenomenon (e.g., non-equilibrium chemical processes) beyond just pure turbulent flow aerodynamics.
 - In order to isolate model-form discrepancies, the validation process should be performed using a UQ-centric framework.

- **Quantifying model adequacy requires some form of “truth” data.**
 - When in the form of measurements, this usually precludes a direct validation of the term being modeled and the model itself.
 - When in the form of higher-fidelity data (e.g., DNS), the validation can typically only be performed in simplified (or idealized scenarios).



- **Other considerations:**
 - Separating model form errors from other uncertainty sources (e.g., imprecise or partially known BCs).
 - Accounting for numerical artifacts (e.g., discretization error).
 - Validation should be performed over as much of the application space as possible.



- **Model validation should involve an assessment of model adequacy considering other uncertainties.**
 - Uncertainties in boundary conditions (typically only an issue if measurements are used to provide the truth data).
 - Numerical errors ... relatively straight forward for RAS, but problematic for SGS closures.
- **Probability Box approach can be used for this purpose.**
 - Aleatoric and Epistemic uncertainty sources are treated separately.
 - Aleatoric uncertainties are irreducible and inherently random, and are typically described by PDFs.
 - Epistemic uncertainties are systematic uncertainties that are a result of inadequate knowledge ... these sources of uncertainty can in principle be reduced if further knowledge is gained.
 - Reference: Roy and Oberkampf, “Computational Methods in Applied Mechanics and Engineering,” Vol. 200:25, 2011, pp. 2131-2144.

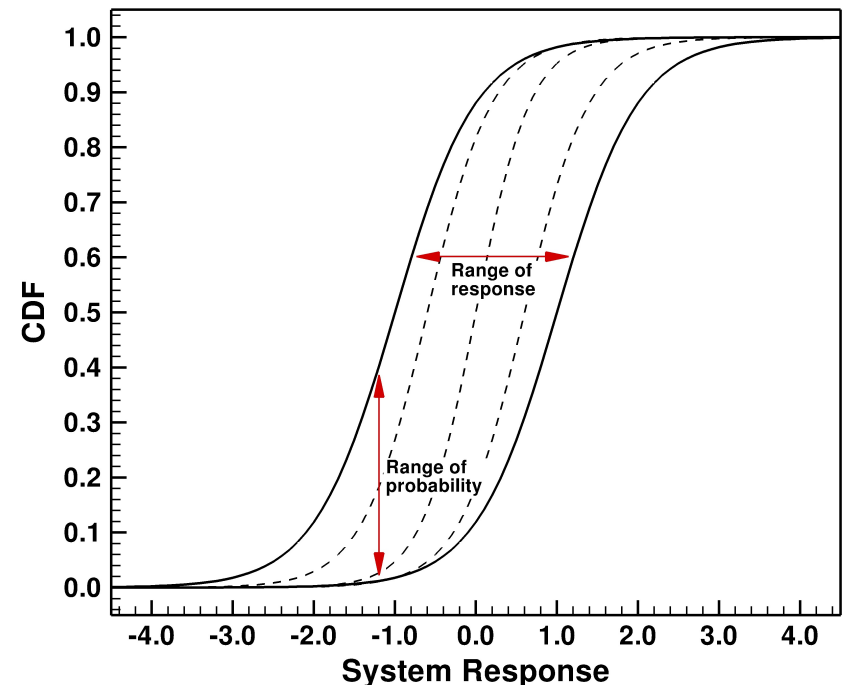
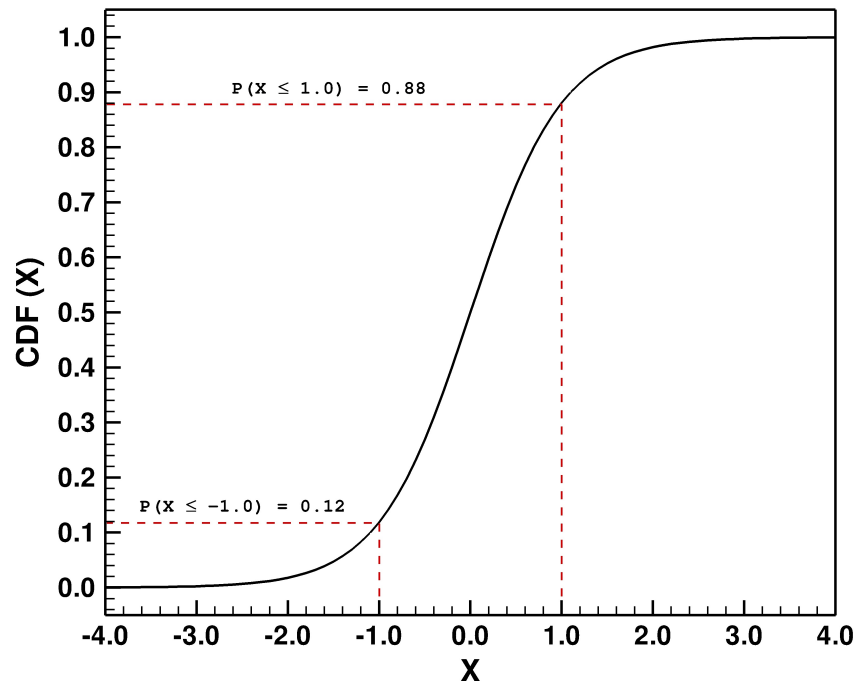
P-Box Uncertainty Quantification Framework



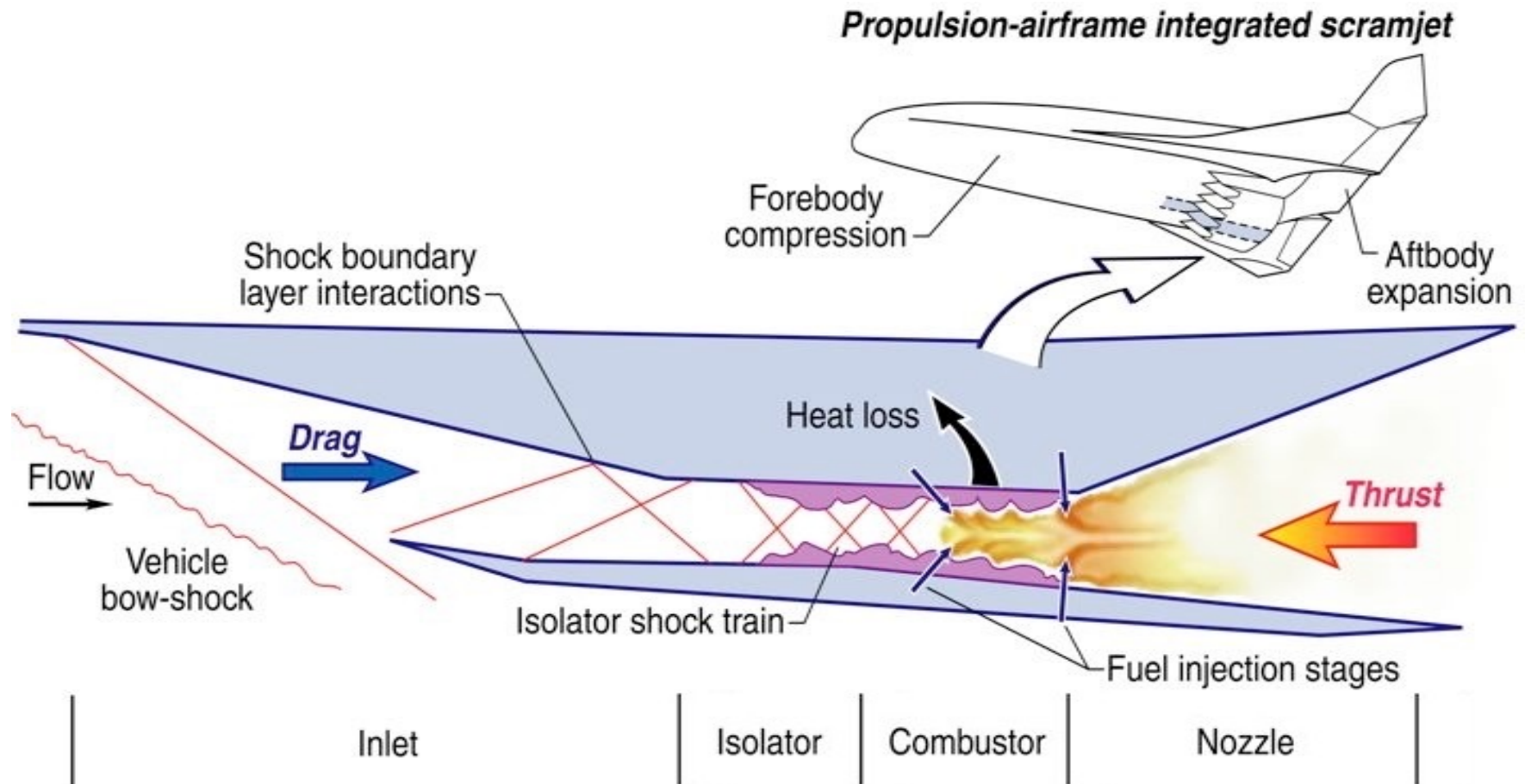
Steps in the UQ process:

- (1) Identify and characterize each uncertainty (aleatoric or epistemic)
- (2) Prioritize the sources of uncertainty
- (3) Propagate the uncertainties through the “computational model” to extract the QoI

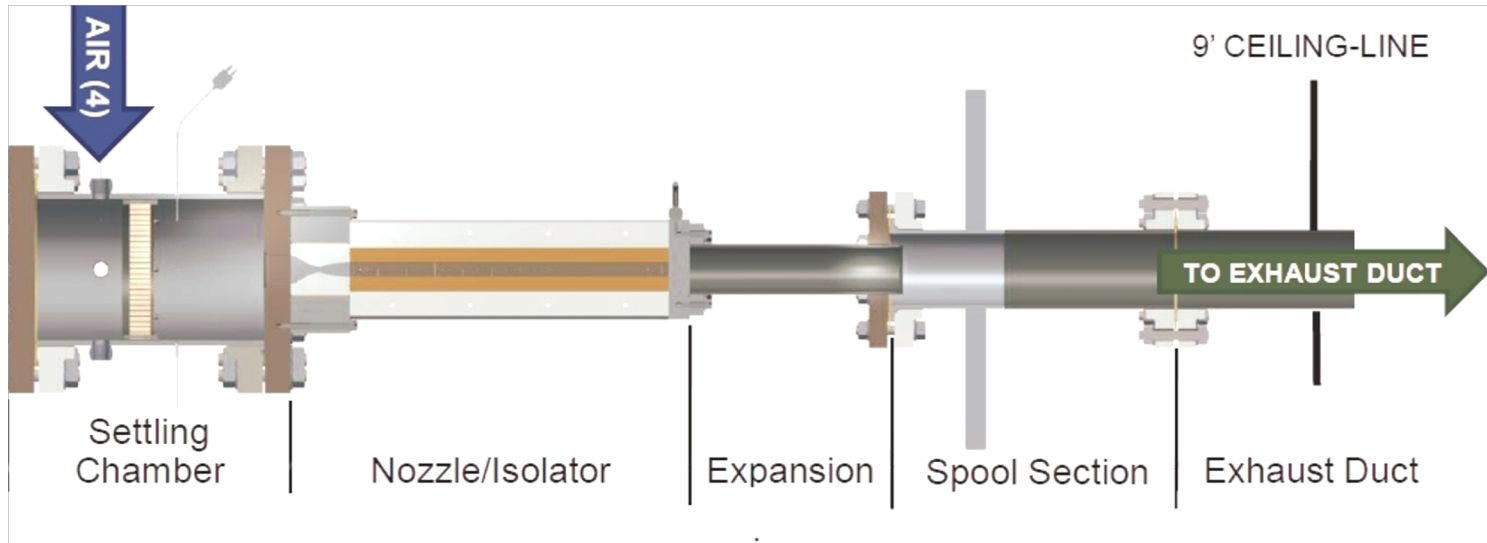
```
Do n = 1, Ne  
  Do m = 1, Na  
    evaluate QoI  
  End Do  
End Do
```



Validation with Uncertainty Example for RAS



Validation with Uncertainty Example for RAS



- **Step 1: Identify and characterize potentially important uncertainty sources**
 - Spatial discretization error (EPISTEMIC)
 - Onset of laminar to turbulent transition (EPISTEMIC)
 - Facility supply pressure (ALEATORIC)
 - Facility supply temperature (ALEATORIC)
 - Facility supply turb. intensity (0.01% to 5%, EPISTEMIC)
 - Facility wall temperature (room variability, EPISTEMIC)
 - Isolator exit pressure (ALEATORIC)



- **Step 2: Retain only those sources that are deemed most sensitive to the QoI**
 - A local sensitivity analysis was undertaken here via one-at-a-time variations of each uncertainty source.
 - Spatial discretization error (EPISTEMIC)
 - Onset of laminar to turbulent transition (EPISTEMIC)
 - Facility supply pressure (ALEATORIC)
 - Isolator exit pressure (ALEATORIC)
 - Moreover, a correlation between facility supply pressure and isolator exit pressure allowed these uncertainties to be combined as one.

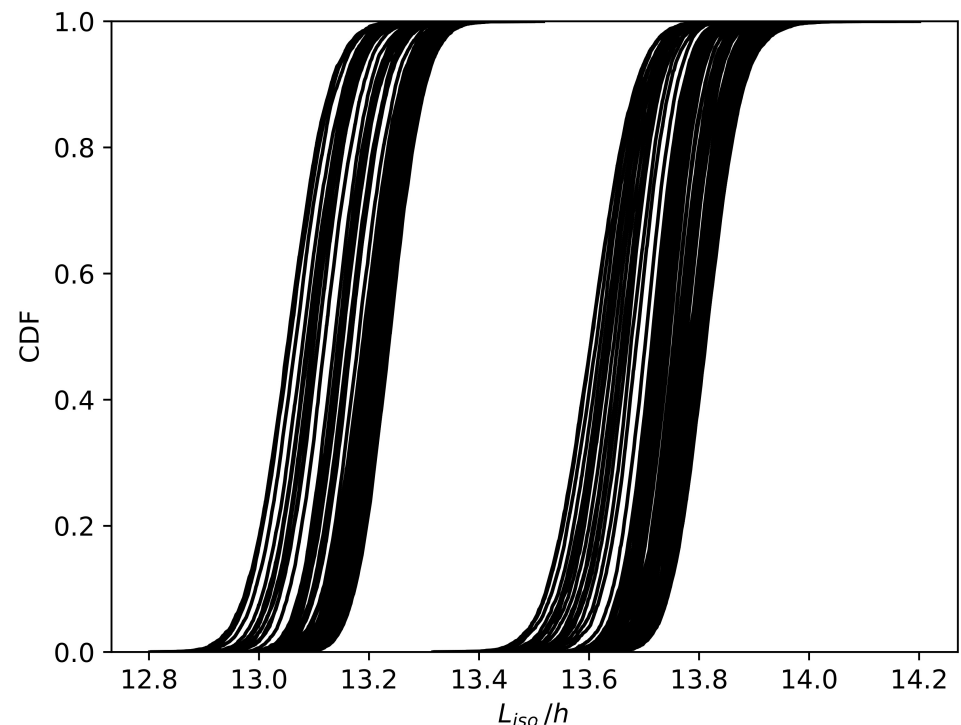
Validation with Uncertainty Example for RAS



- **Step 3: Propagate the uncertainties to establish the uncertainty in the Qol (shock train length)**
 - Metamodel built for Qol → key cost saving step!
 - Total of 14 CFD simulations (6 medium and 8 coarse grid)

```
Do n = 1, Ne  
  Do m = 1, Na  
    evaluate Qol  
  End Do  
End Do
```

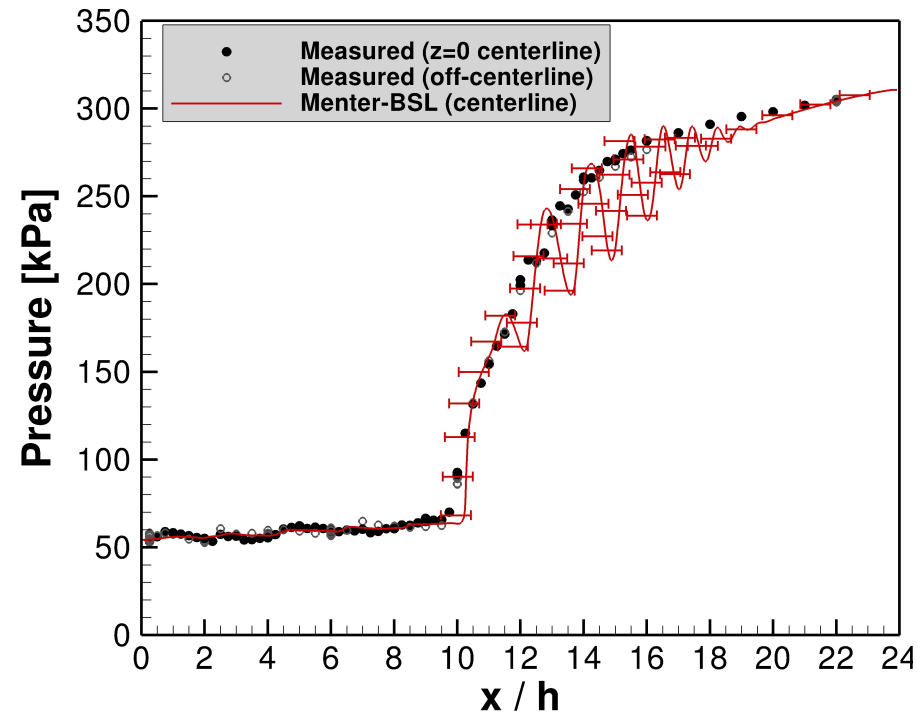
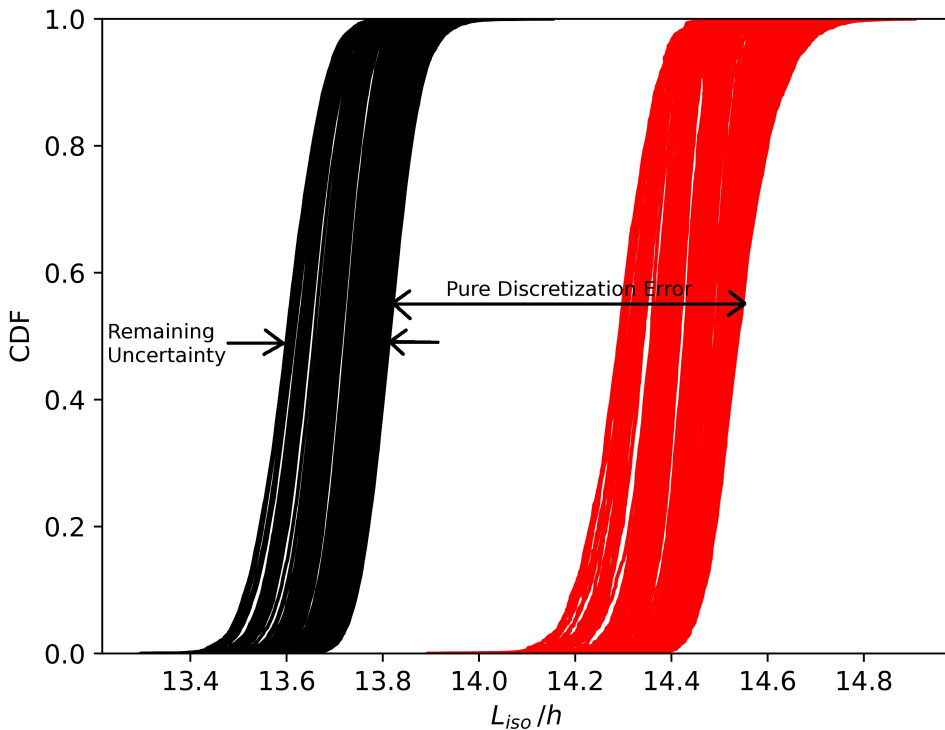
- The probability box shown here defines the range of shock train length predictions given the uncertainty in facility pressure ratio, transition onset, and grid level.



Validation with Uncertainty Example for RAS



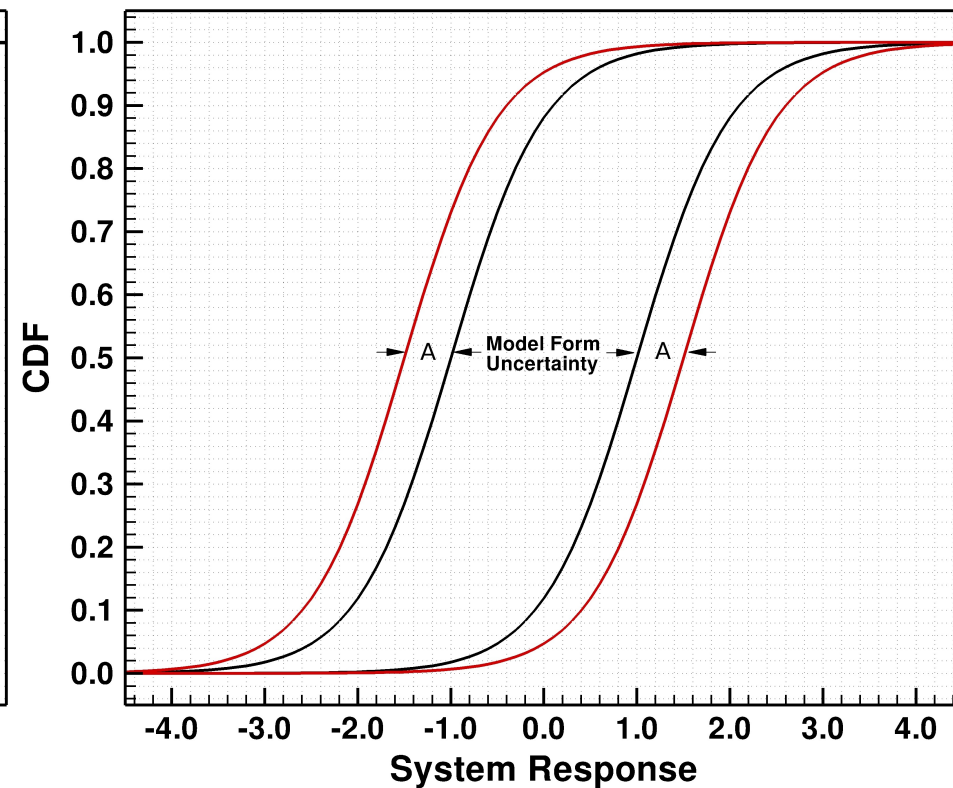
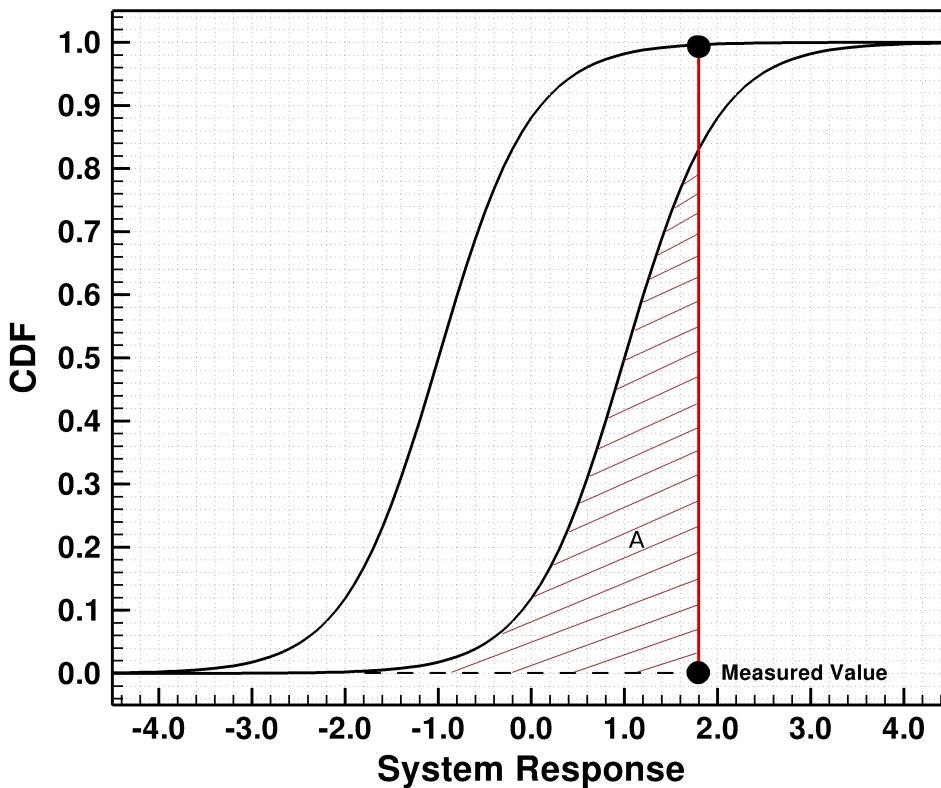
- The UQ information can also be displayed in a more conventional manner as error bars.
 - Discretization error is known to be a one-sided bias error (if asymptotic convergence demonstrated).
 - Remaining error is equally distributed on the uncertainty bar.



Determination of Model-Form Uncertainty



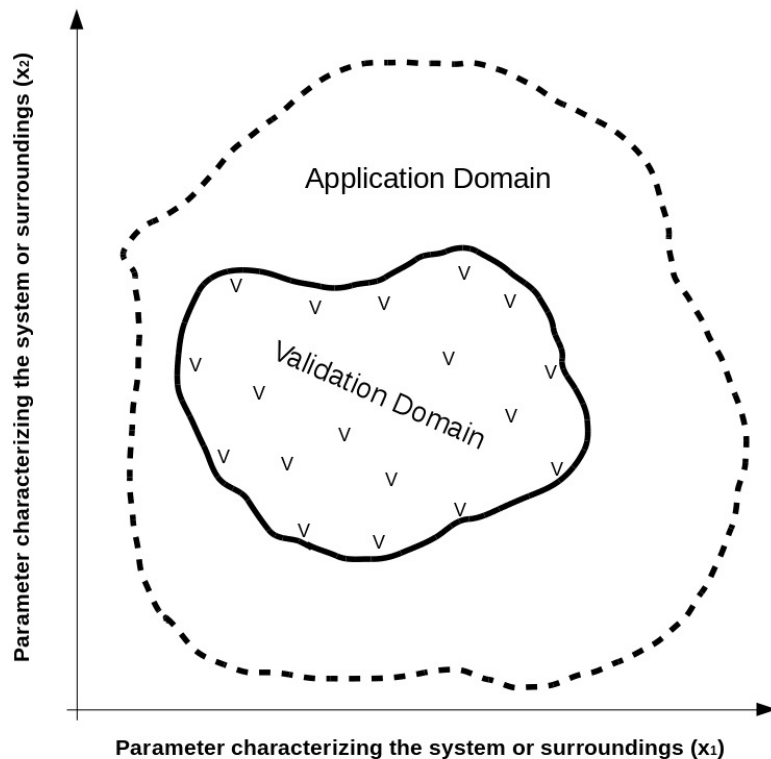
- Any discrepancy between the model and "truth" can now be quantified taking into account other sources of uncertainty.
 - The area validation metric is often used for this purpose.



Determination of Model-Form Discrepancy



- To complete the turbulence closure validation, the process just described needs to be repeated over as much of the application domain as possible.



- Once the validation domain has been populated, a metamodel is built for the model discrepancy based on the area validation metric.
- The model form discrepancy can now be extracted from this metamodel at any condition of interest to pad the probability box of future predictions.

Complication with SGS Model Validation



- **Model-form errors can be assessed independently of discretization errors for RAS.**
 - Previous example illustrated how to assess model-form discrepancy in the presence of simulation uncertainties and numerical discretization error.
- **In LES, a filter width appears explicitly in SGS closures → typically defined by some measure of the grid spacing.**
 - This entangles the SGS model-form and numerical errors.
 - Implies grid independence only when close to DNS resolution.
 - No guarantee that numerical error and SGS closures scale at the same rate with refinement (hard to imagine any real-world scenario where this can be claimed).

Complication with SGS Model Validation



- **What to do?**
 - Accept the numerical and model-form error as a single error source.
 - Downside is that the discrepancy quantified in ground tests can't be untangled from the SGS closure error ... not clear how to reliably use ground test knowledge to estimate model-form error for future predictions.
 - Moreover, numerical scheme truncation error and aliasing error can dominate the contribution of the subgrid closure.
 - Fix the filter width ($\Delta = C \cdot h_0$) and refine the grid ($h_2 < h_1 < h_0$) until the discretization error estimate is deemed small enough.
 - Allows some separation of model discrepancy and numerical error.
 - Downside is additional expense incurred without the natural reduction of model-form error with grid refinement fully realized.
 - Explicitly filter the equations in order to separate the filtering and discretization operators.
 - Allows a path towards true grid independent solutions → implying that any discrepancy with the filtered DNS can be attributed solely to the SGS closure.
 - Lots of caveats here (filter commutation with differentiation, cost, ...).
 - True grid independence is not necessarily required within a UQ framework.



- Pope, S., “Ten Questions Concerning the Large-Eddy Simulation of Turbulent Flows,” New Journal of Physics, Vol. 6, No. 1, 2004.
 - Classical article describing the various “warts” with LES
- Bose, S. T., Moin, P. and You, D. “Grid-independent large-eddy simulation using Explicit Filtering,” Center for Turbulence Research Annual Research Briefs, 2008.
 - Compressible extension provided in 2010
- Model Validation for Propulsion (MVP) Workshop (<https://community.aпан.org/wg/afrlwg/mvpws>)
 - Gallagher, T. P. and Sankaran, V., “Affordable Explicitly Filtered Large-Eddy Simulation for Reacting Flows,” AIAA JOURNAL, Vol. 57, No. 2, February 2019.

- **High-fidelity CFD data plays a dominant role in the design/analysis for combustion applications.**
 - Continual desire to rely more on CFD and less on ground testing.
- **A UQ-centric approach to CFD supplies the necessary information for “Risk Informed” decisions.**
 - Confidence in simulation data needs to accompany the raw data.
- **Quantifying model-form discrepancy is essential for CFD to be used as a predictive tool.**
 - Benchmark applications need to be performed in a UQ-centric fashion to help the end user choose the “best” model for the chosen application
 - For SRS, the best model judged by cost required to achieve acceptable accuracy.
- **Scale-resolving simulations introduce a complication of entanglement of numerical error and model-form error.**
 - Fixed filter width with grid resolution (or possibly explicitly filtered approaches) likely required to quantify model form discrepancy.

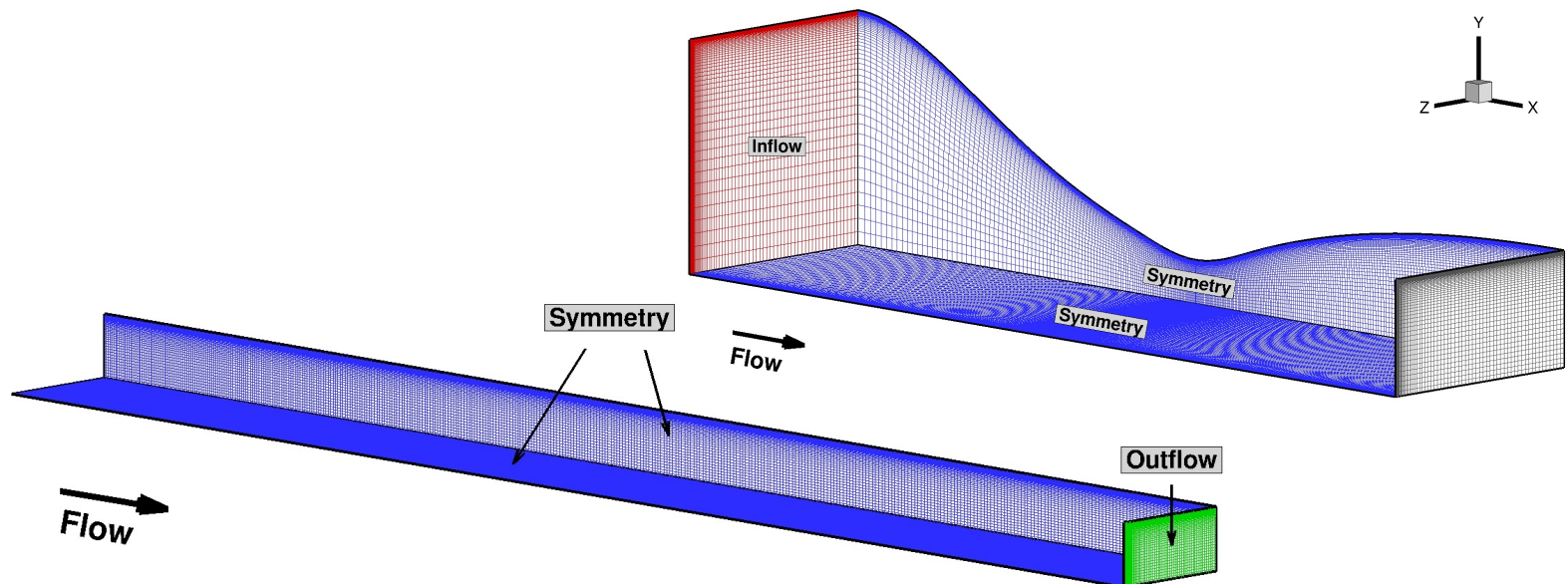
Back-up Slides ...



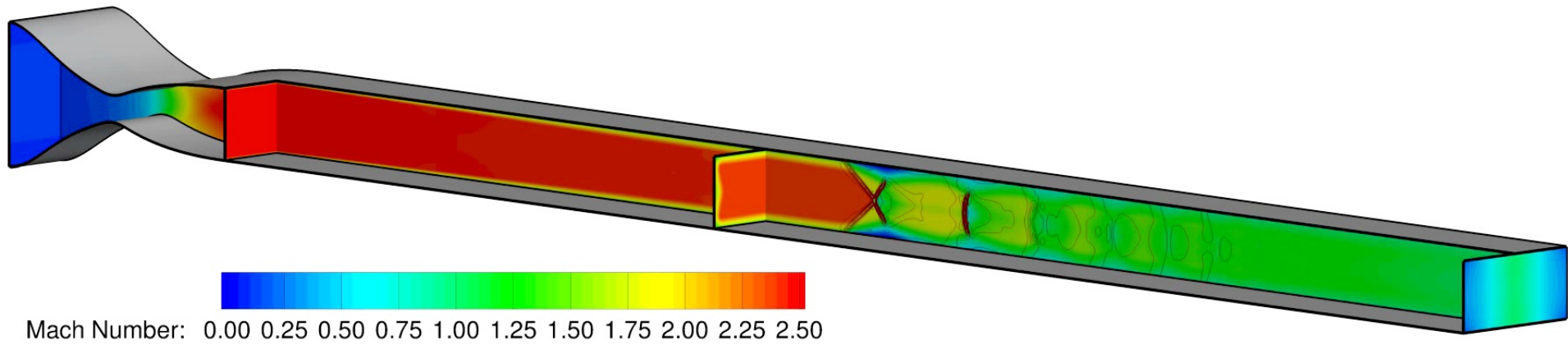
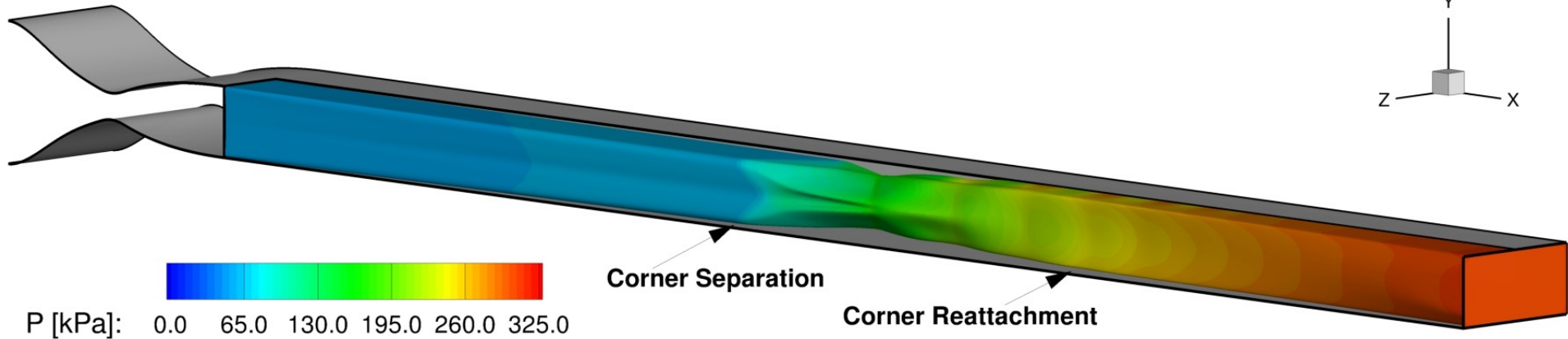
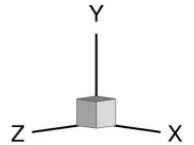
Simulation Description



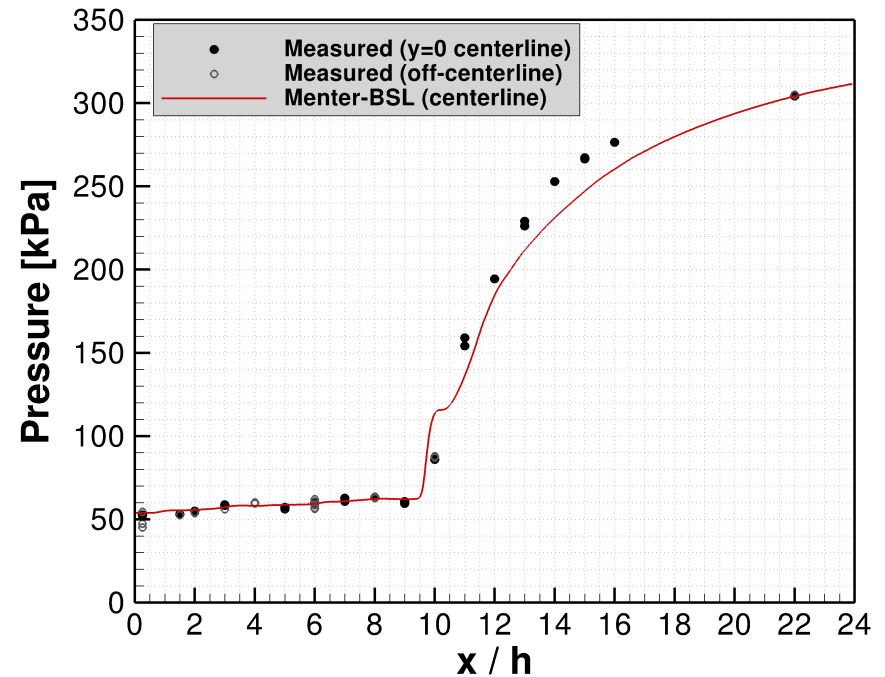
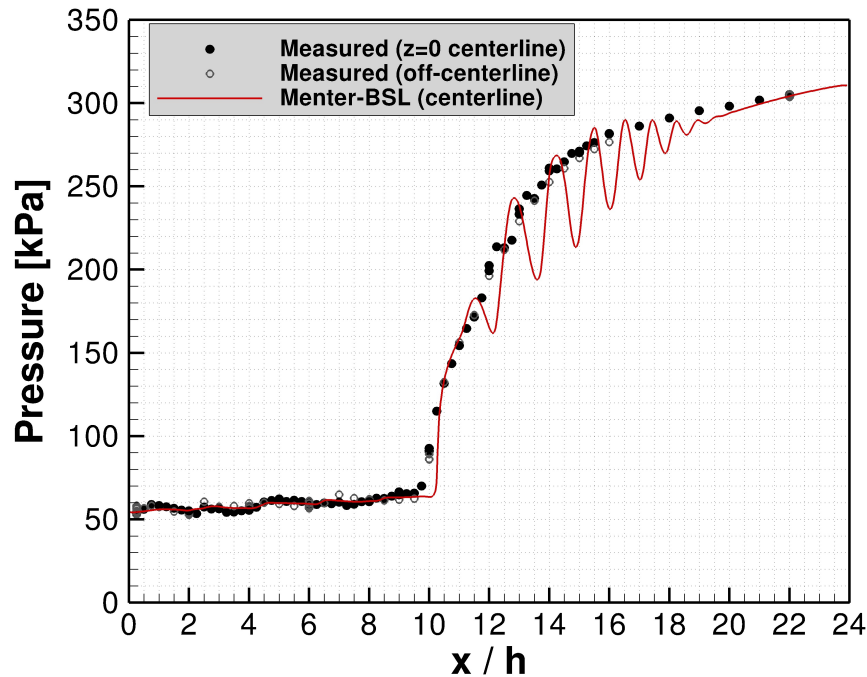
- **Reynolds-averaged simulations performed with VULCAN 7.0**
 - Menter-BSL $k-\omega$ model chosen for the turbulence closure model
 - All solid surfaces specified as no-slip adiabatic walls
 - Back-pressure specified from measurements
 - Nozzle inflow conditions specified via stagnation properties
 - 3 grid levels (2000 x 160 x 208), (1000 x 80 x 104), (500 x 40 x 52)



Isolator Flowfield Description



Nominal Comparison with Measurements



- **Observations:**

- Measurements show a monotonic pressure rise, simulations do not
- Shock train length (QoI) appears to be well predicted on both surfaces

- **What confidence do we assign to this prediction?**

- Multiple uncertainties exist that can impact the simulation predictions
- Separation of model performance from other uncertainty sources is required to make definitive claims of model-form adequacy



- **Step 3a: Build a metamodel for Qol for the uncertainty propagation**
 - Key cost-saving step since the direct use of 3-D CFD for uncertainty propagation would be impractical.
 - Design space used to construct the metamodel based on bounding estimates of each uncertainty variable:
 - Facility pressure ratio spanned the range of values given by the nominal value $\pm 3\sigma$ (Gaussian).
 - Onset of transition assumed to take place between the nozzle entrance and the inflection point downstream of the throat.
 - Spatial discretization treated as a categorical uncertainty using the medium and coarse grid levels.
 - A total of 14 CFD simulations (6 medium grid and 8 coarse grid) were used to define the metamodel.
 - An evaluation of the metamodel fit adequacy was performed and the metamodel prediction error was included as an aleatoric uncertainty.

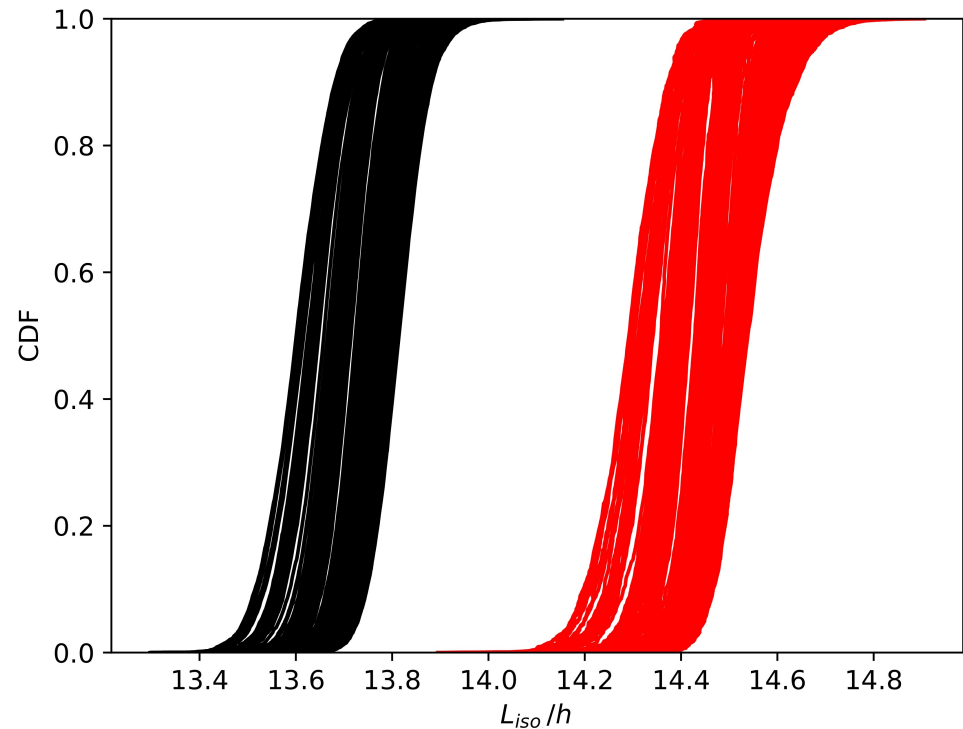
Validation with Uncertainty



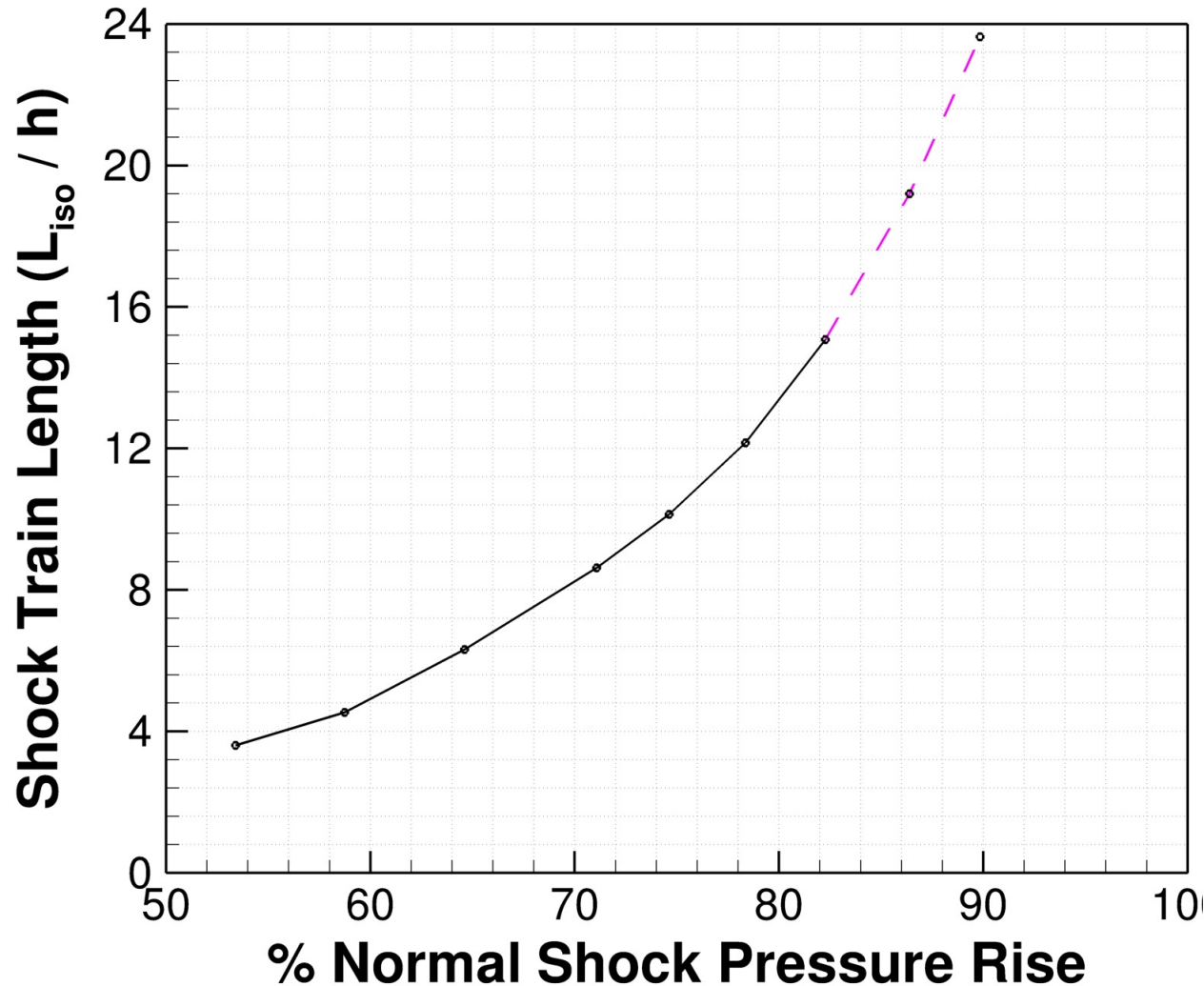
- Transformation of grid level uncertainty to a measure of discretization error

$$\text{GCI} = F_s \frac{|f_2 - f_1|}{r^p - 1}$$

$$L_{iso}^* - L_{iso2} = F_s \frac{L_{iso2} - L_{iso1}}{r^p - 1}$$



Shock Train Sensitivity to Back-Pressure



Metamodel Adequacy of Fit



R^2_{adjusted} : An adequacy measure similar to the correlation coefficient but includes penalties for the number of modeling terms used (ideally it should be 0.99 or larger).

$R^2_{\text{predicted}}$: A cross-validation metric that removes one fit point from the metamodel at a time and refits the metamodel, essentially validating it against points used to fit the model (ideally it should be close to **R^2_{adjusted}** to provide model stability confidence).

