2021 HPCMP User Group Meeting, September 21-23, 2021

A Practical Approach to Uncertainty Quantification Using Probability Boxes

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Assessing the Credibility of CFD Results

- **Flight vehicle design/analysis relies heavily on CFD.**
  - Trend is an ever increasing reliance on numerical data
    - Limitations (environment, scale, and duration) of ground test facilities
    - Advanced diagnostics are more difficult in full-scale facilities
  - Increased pressure to simulate more and test less
- **How good are these CFD simulations?**
  - Confidence (or lack there of) in the results is rarely communicated
  - Instead a deterministic simulation strategy is the state-of-practice
    - Typical goal is to maximize the coverage of the design space (e.g., increase resolution of aero-databases)
  - Can this culture continue to be justified?
- **A UQ-centric approach to CFD can provide "Risk Informed" decisions.**
  - Confidence in simulation data should accompany the raw data

Barriers Preventing Incorporation of UQ

- **Why is UQ not commonly a standard practice in the CFD workflow?**
  1) The CFD applicationist is often not well versed with UQ methods
     - UQ is its own complex scientific discipline, so standard "Joe" engineer may not know how best to incorporate it
  2) Workload of the CFD applicationist is inevitably increased
     - Preparation of "n" simulations instead of 1 deterministic one
  3) Increase computational cost
     - 1 deterministic simulation replaced with "n" simulations

- **Through automation, the first 2 items can be eliminated as barriers.**
- **The last barrier is addressed by the flexibility offered in the statistics package used.**
  – Goal is to keep "n" as small as possible (e.g., surrogate modeling)

Uncertainty Quantification Framework

- **Desired UQ framework attributes:**
  - Nonintrusive (no modifications required to CFD tool)
  - Computationally inexpensive (in a relative sense)
  - Retain the core features emphasized by the UQ community
  - Ability to automate the process

- **Probability Box approach**
  - Aleatoric and Epistemic uncertainty sources are treated separately.
  - Aleatoric uncertainties are irreducable 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.

Uncertainty Quantification Framework

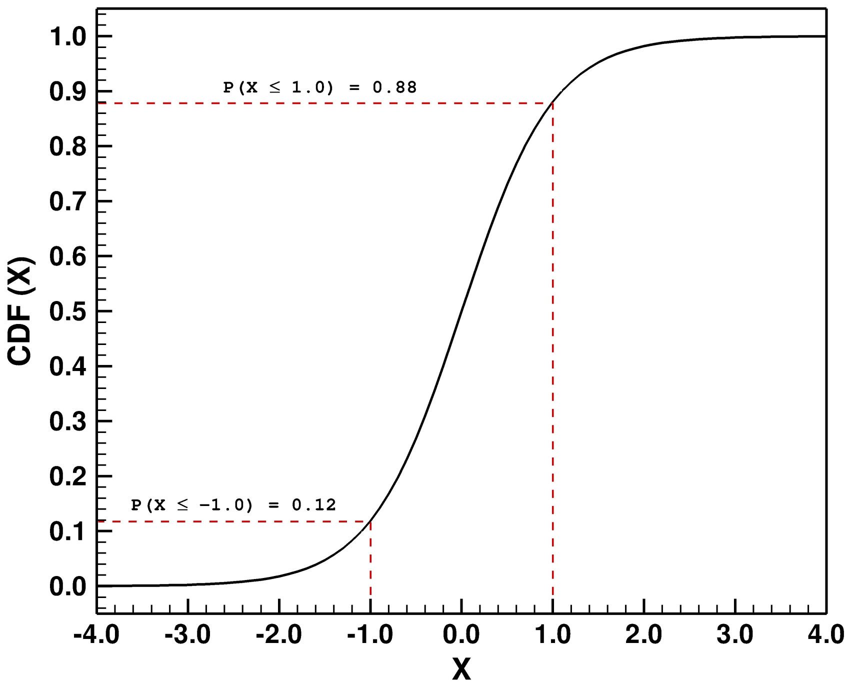
Steps in the UQ process:

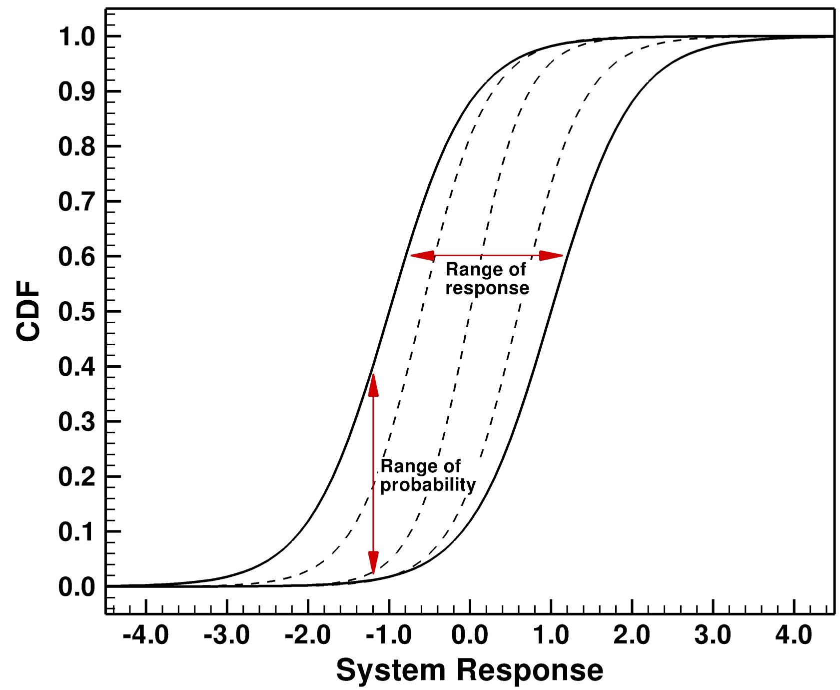
(1) Identify and characterize each uncertainty

(2) Prioritize the sources of uncertainty

(3) Propagate the uncertainties through the "computational model" to extract the QoI

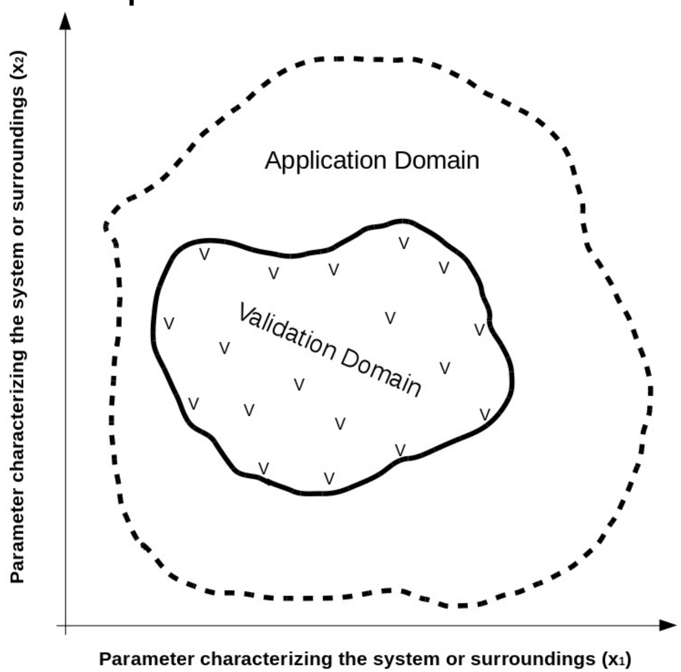
```
Do n = 1, N_e
   Do m = 1, N_a
      evaluate QoI
   End Do
End Do
```





Application of UQ: Turbulence Model Validation

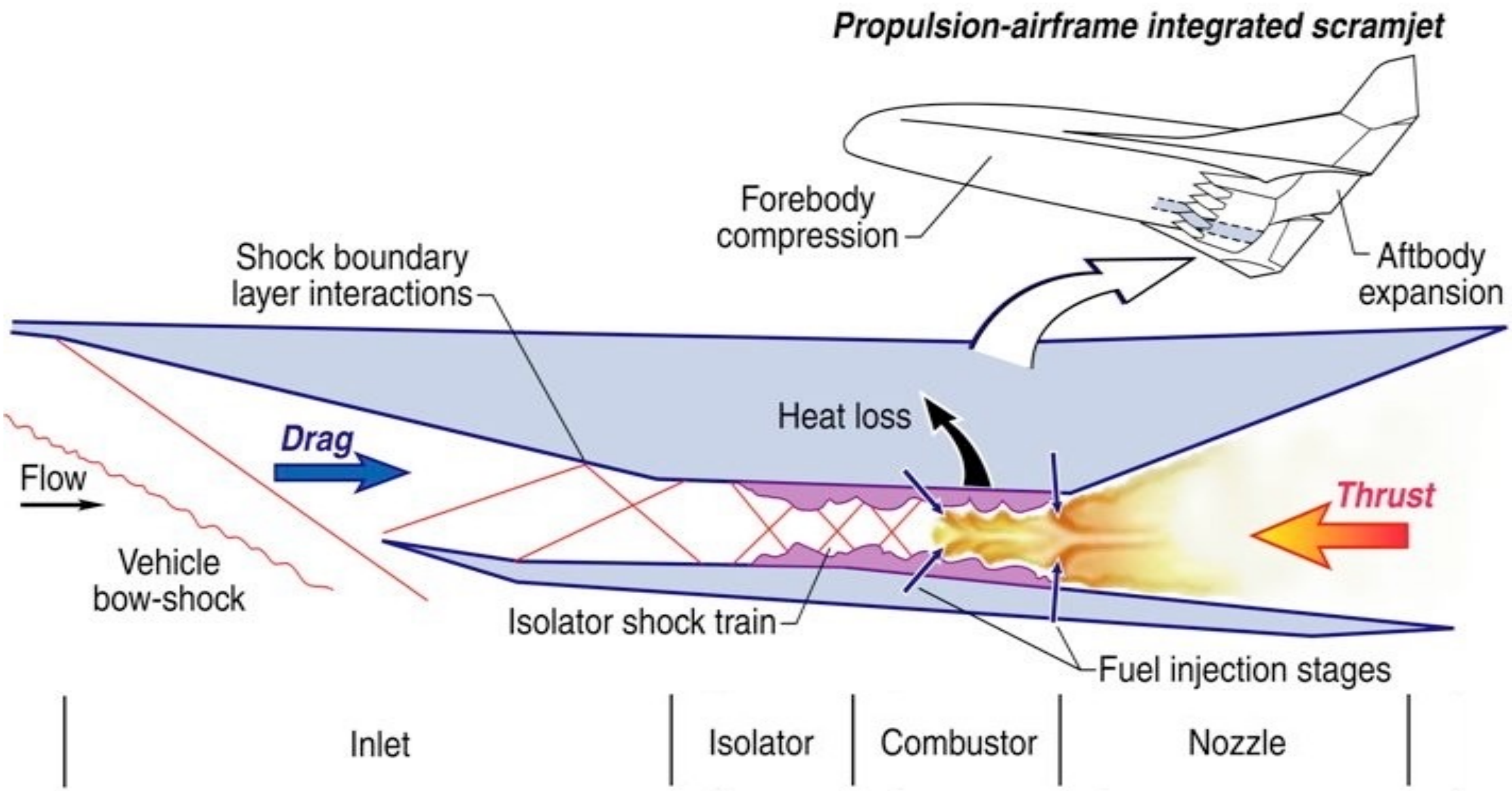
- A significant source of uncertainty in Reynolds-Averaged Simulations (RAS) is the turbulence model closure for the Reynolds stress tensor
  - Model form errors are almost always epistemic (i.e., they represent some sort of bias between the model prediction and the observed physics)
  - Quantifying the uncertainty (bias error) requires a substantial CFD/ground test campaign to map out the errors over as much of the application space as possible



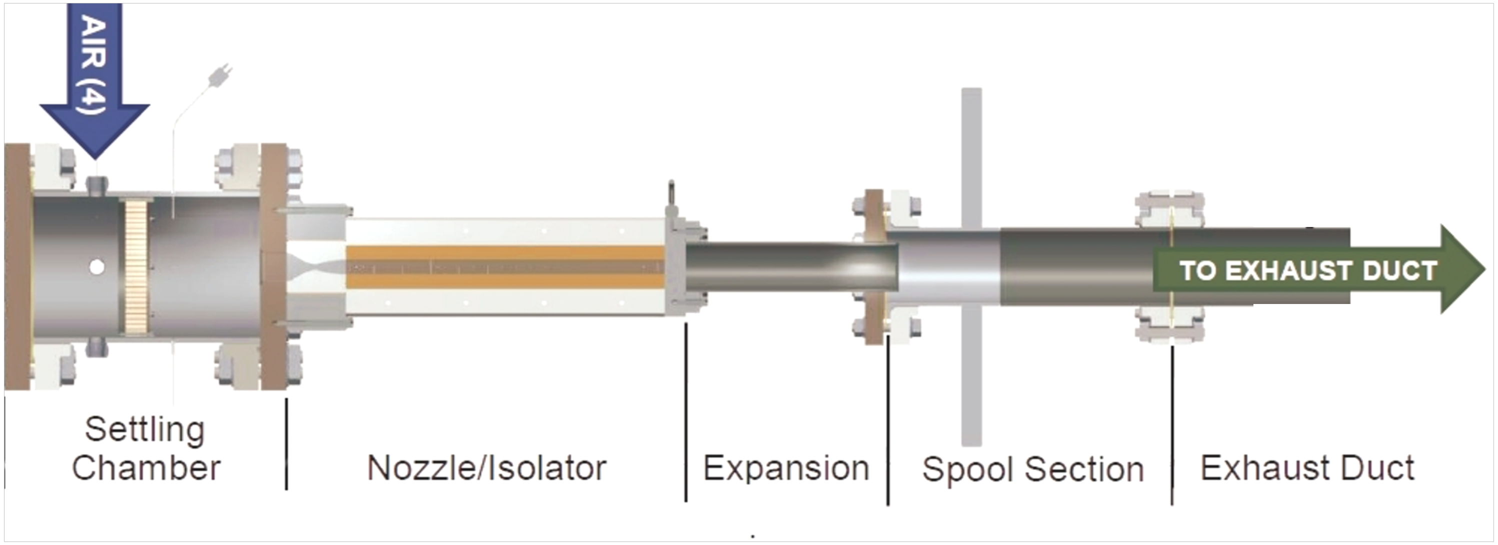
At the vehicle level, this implies that the validation process be performed over the range of conditions that the vehicle might encounter.

How does one determine the model-form discrepancy for use in the UQ process just described?

Scramjet Engine Flow Features …



IDRL Facility Description and Conditions

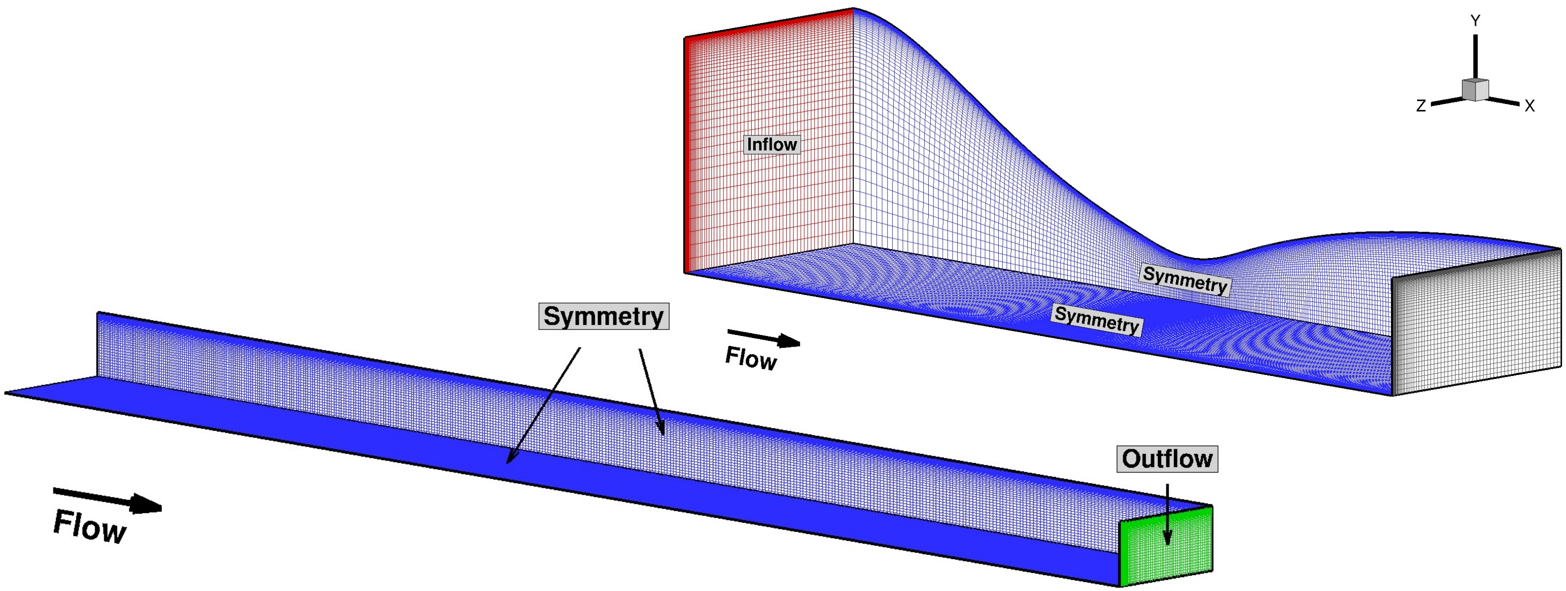


Facility Property	Operating Condition
Nozzle Plenum Pressure [kPa]	908.7* (0.027)
Nozzle Plenum Temperature [K]	292.9 (0.023)
Nozzle Exit Mach Number	2.5*
Nozzle Exit Pressure [kPa]	53.9
Isolator Exit Pressure [kPa]	311.6 (0.097)

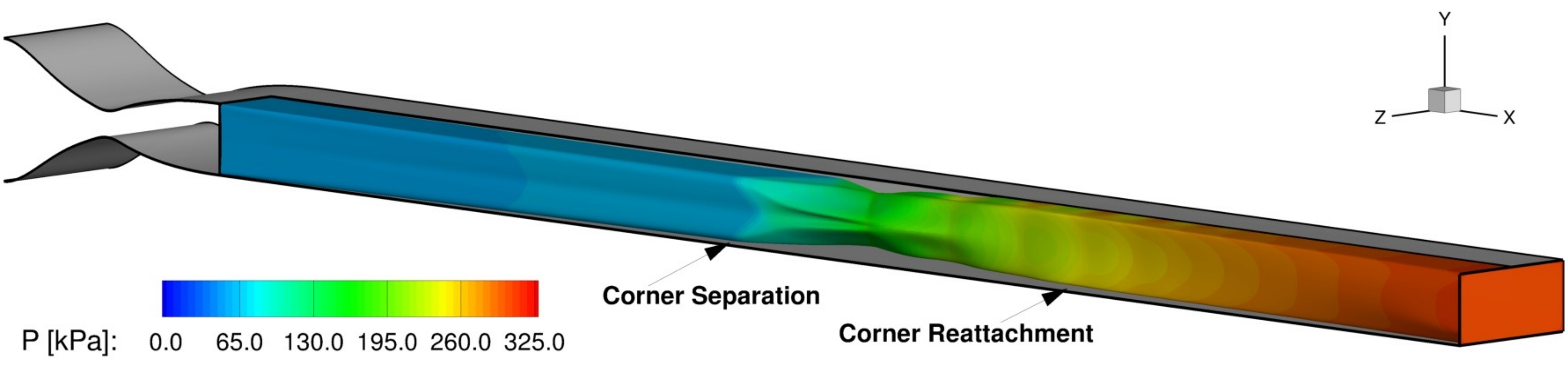
* Nominal value from isentropic relationships

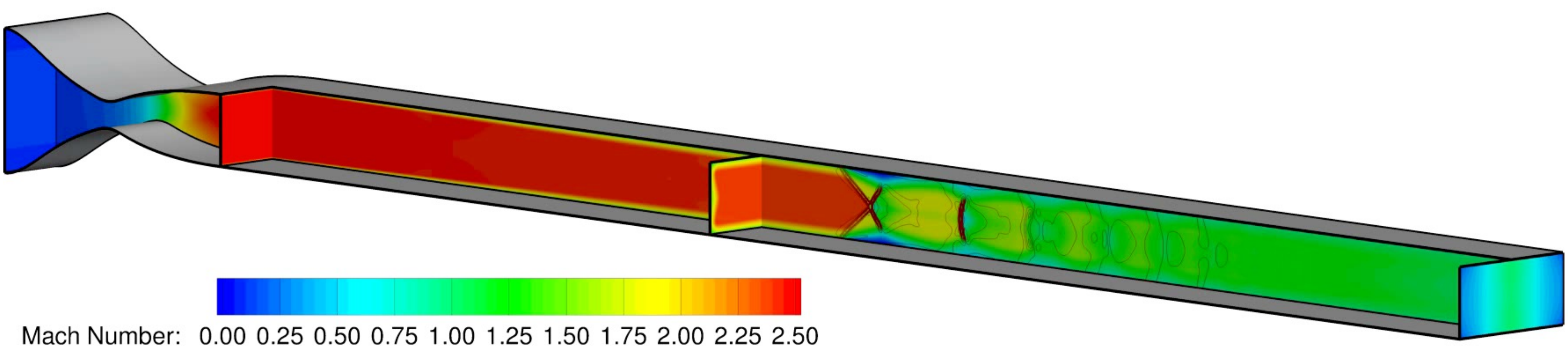
Simulation Description

- **Reynolds-averaged simulations performed with VULCAN 7.0**
  - Menter-BSL k-ω 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)

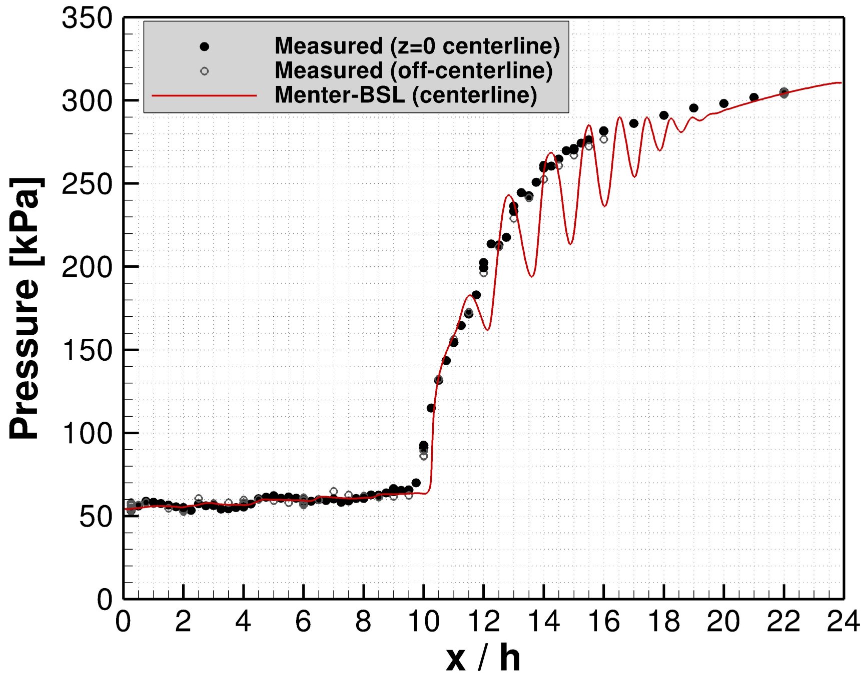


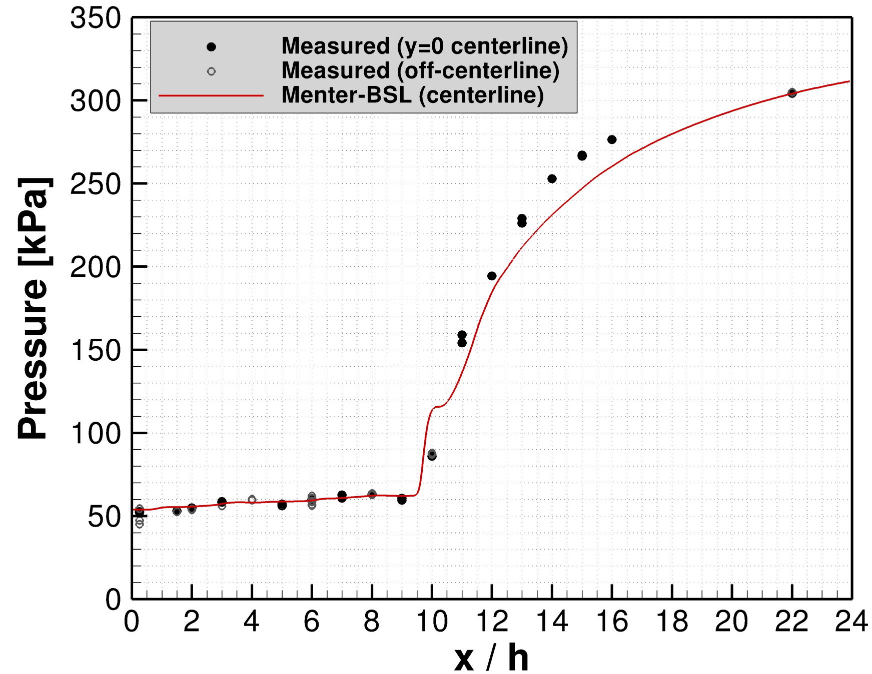
Isolator Flowfield Description





Nominal Comparison with Measurements





- **Observations:**
  - Measurements show a monotonic pressure rise, sumulations 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

Validation with Uncertainty

- **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)

Validation with Uncertainty

- **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

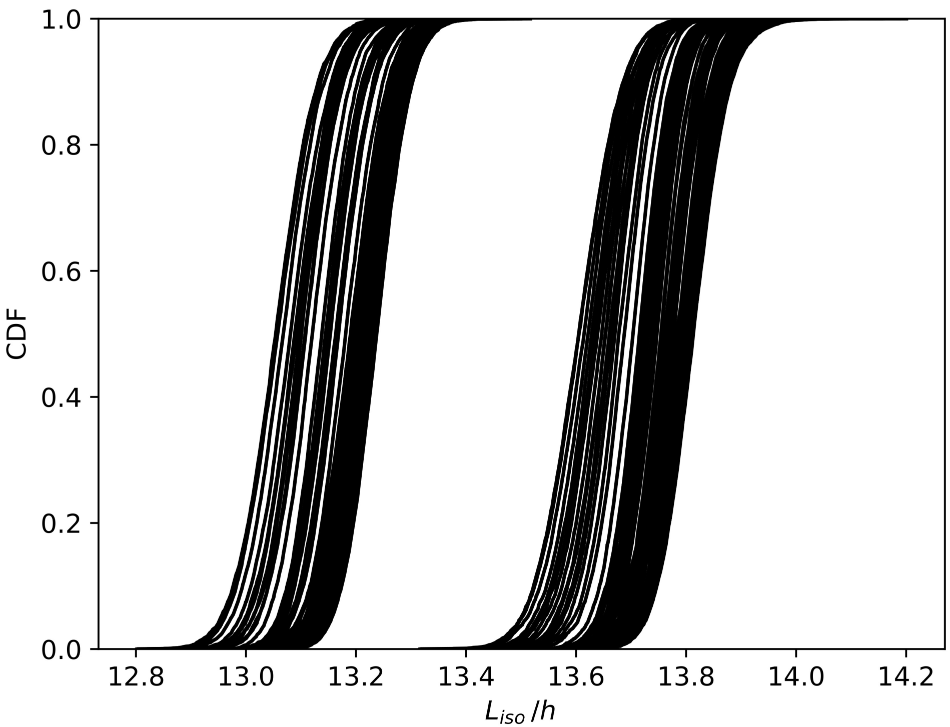
Validation with Uncertainty

- **Step 3a: Build a metamodel for QoI 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 predicition error was included as an aleatoric uncertainty.

Validation with Uncertainty

- **Step 3b: Propagate the uncertainties to establish the uncertainty in the QoI (shock train length):**

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



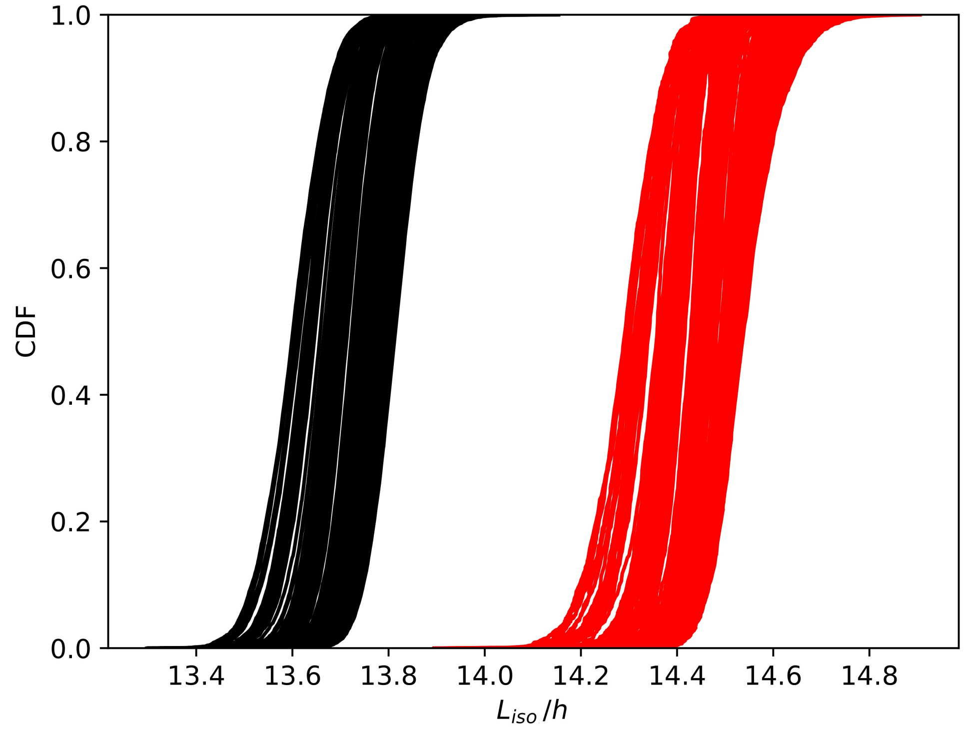
- The probability box shown here defines the range of possible system responses given the uncertainty sources investigated (facility pressure ratio, transition onset, grid level)

Validation with Uncertainty

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

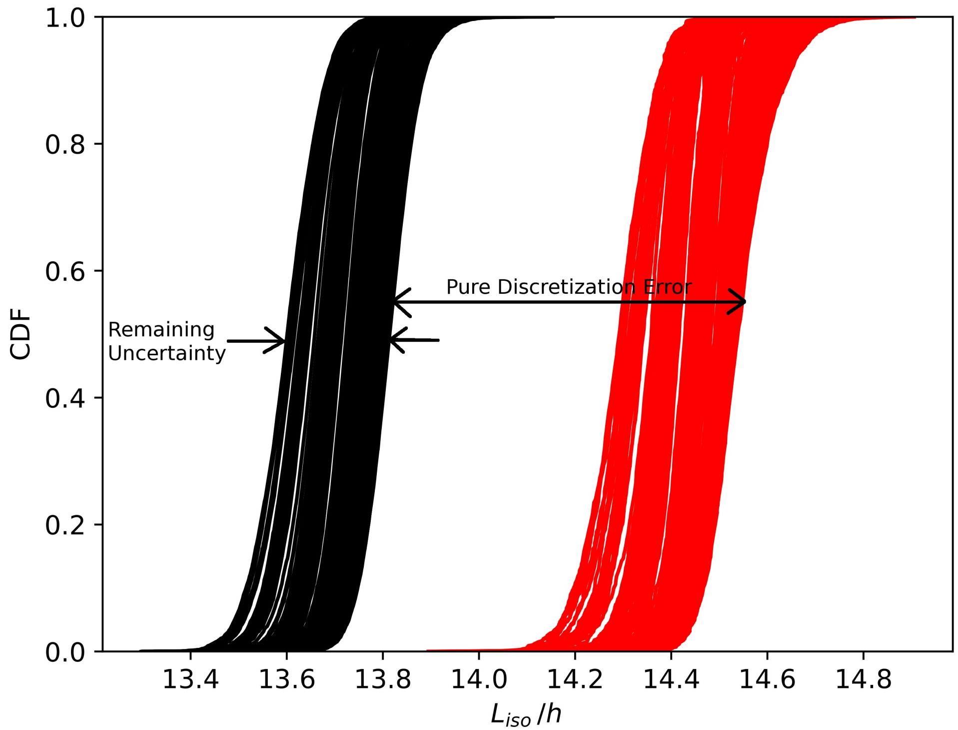
$$\mathrm{GCI} = F_s \frac{|f_2 - f_1|}{r^p - 1}$$

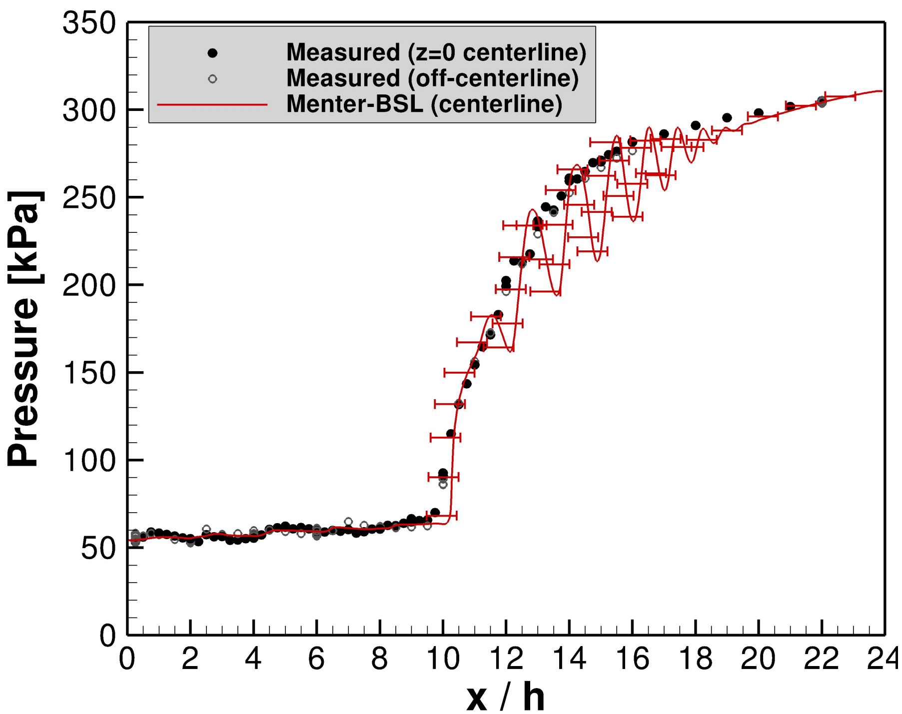
$$\mathrm{L}_{iso^*} - \mathrm{L}_{iso^2} = F_s \frac{\mathrm{L}_{iso^2} - \mathrm{L}_{iso^1}}{r^p - 1}$$



Validation with Uncertainty

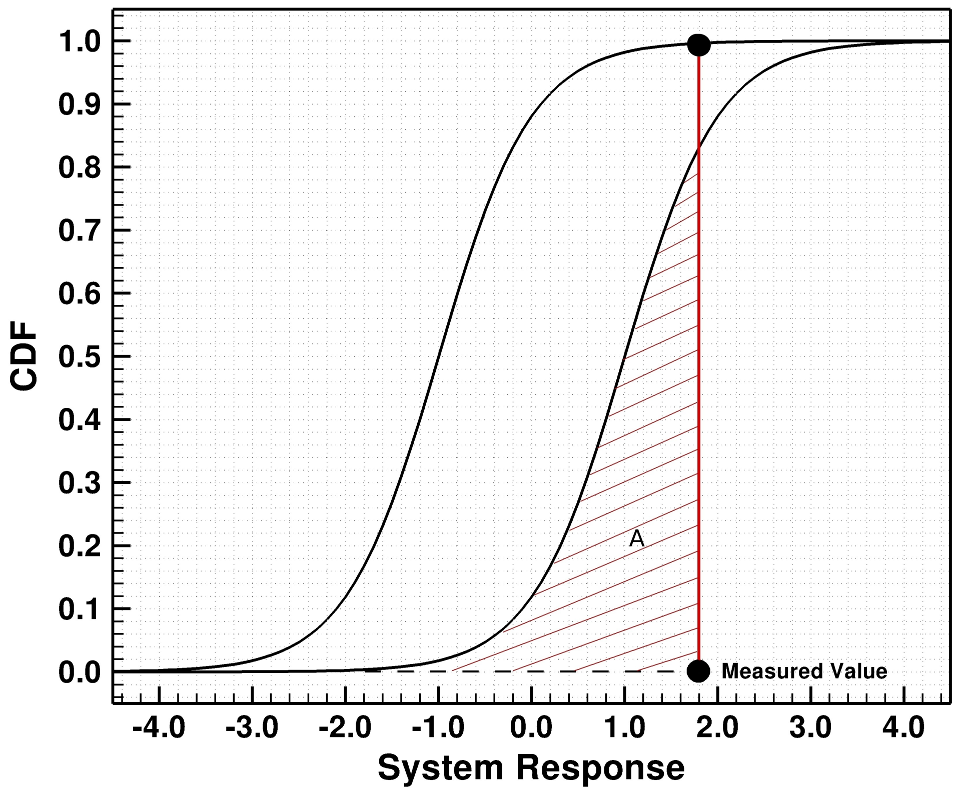
- **The UQ information can also be displayed in a more conventional manner as error bars.**
  - Discretization error is known to be a one-sided bias error
  - Remaining error is equally distributed on the uncertainty bar

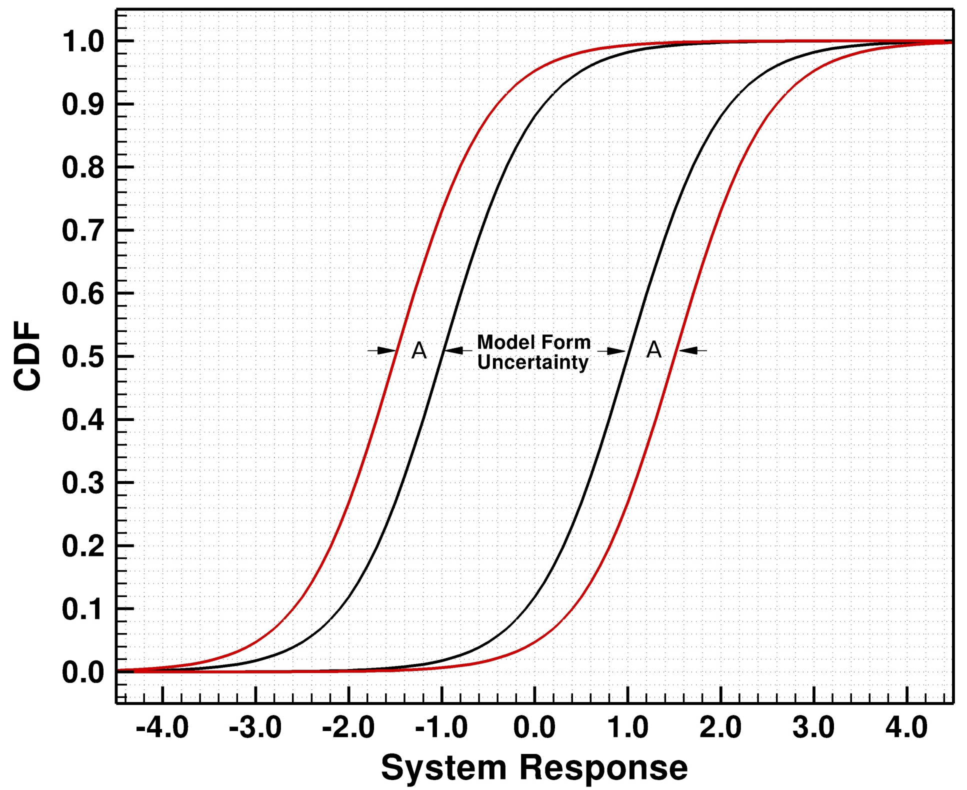




Determination of Model-Form Uncertainty

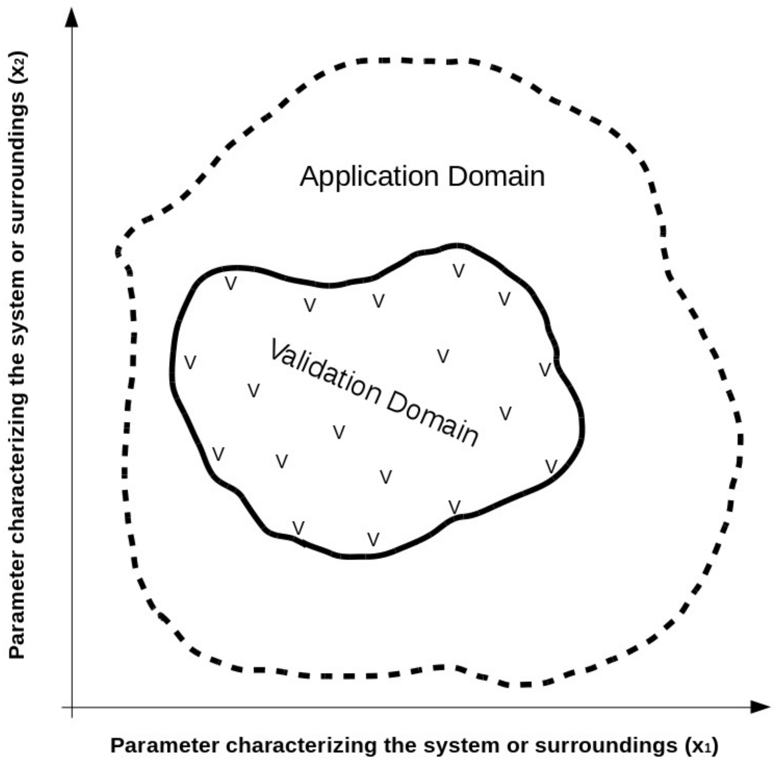
- **To perform a model validation, the process just described should be repeated for all conditions of interest.**
  - Model-form error is quantified by an area validation metric





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**



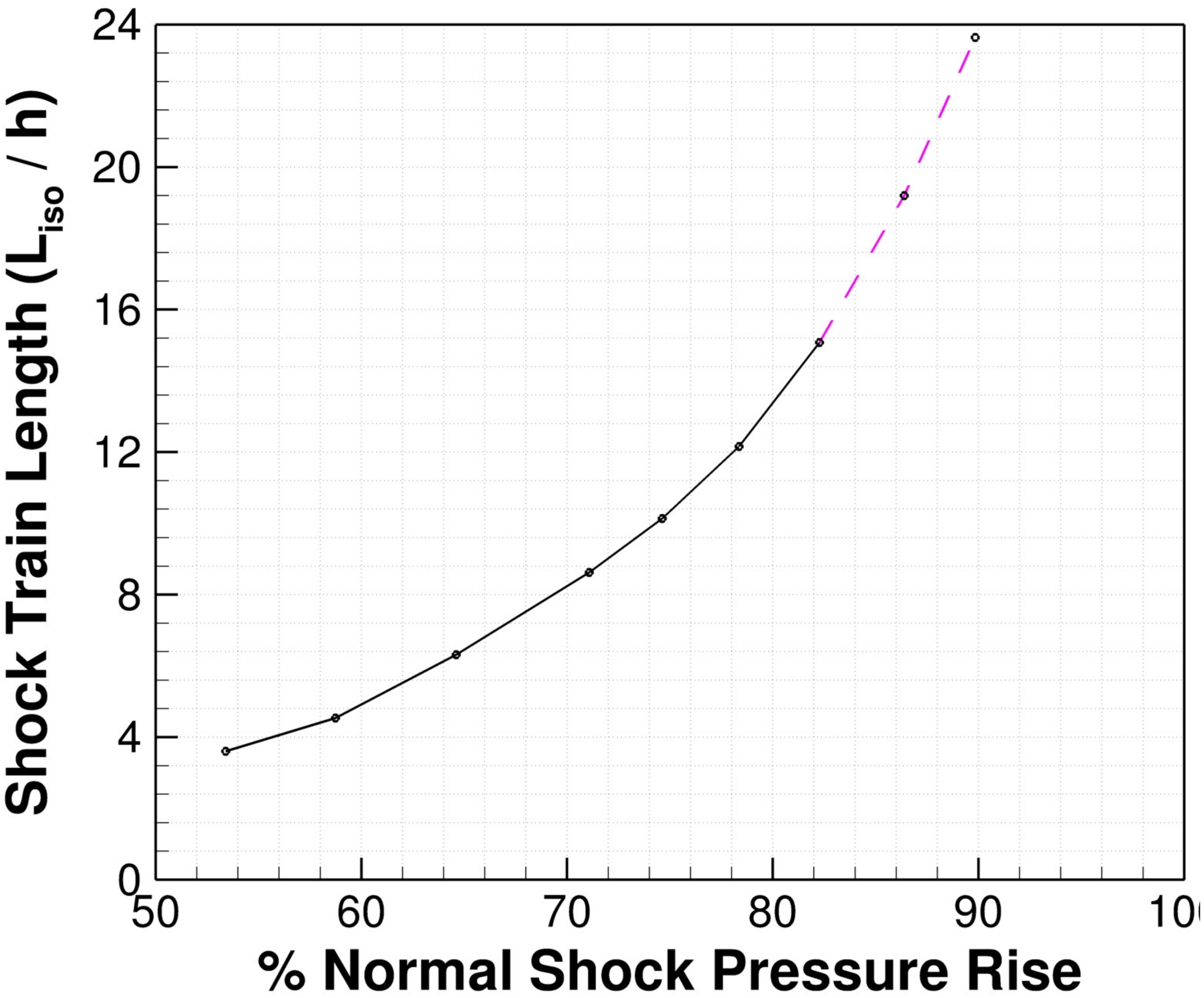
- Once the validation domain has been populated, a metamodel is built for the model discrepancy based on the area validation metric.
- The model form discrepancy can now be extracted from this metamodel at any condition of interest to pad the probability box of future flight predictions.

Summary

- **High-fidelity CFD data plays a dominant role in the design/analysis of aerospace vehicles.**
  - 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.
- **A nonintrusive 2nd-order uncertainty quantification framework has been described that encapsulates the uncertainty information in the form of a probability box.**
  - This information can easily be recast in other forms as desired.
- **Approach was demonstrated in the context of a validation activity.**
- **The cost of performing the uncertainty assessment was reduced to a manageable level through the construction of a metamodel.**
  - Cost was further reduced through the use of coarser grids with the added numerical error included in the uncertainty assessment.

Back-up Slides …

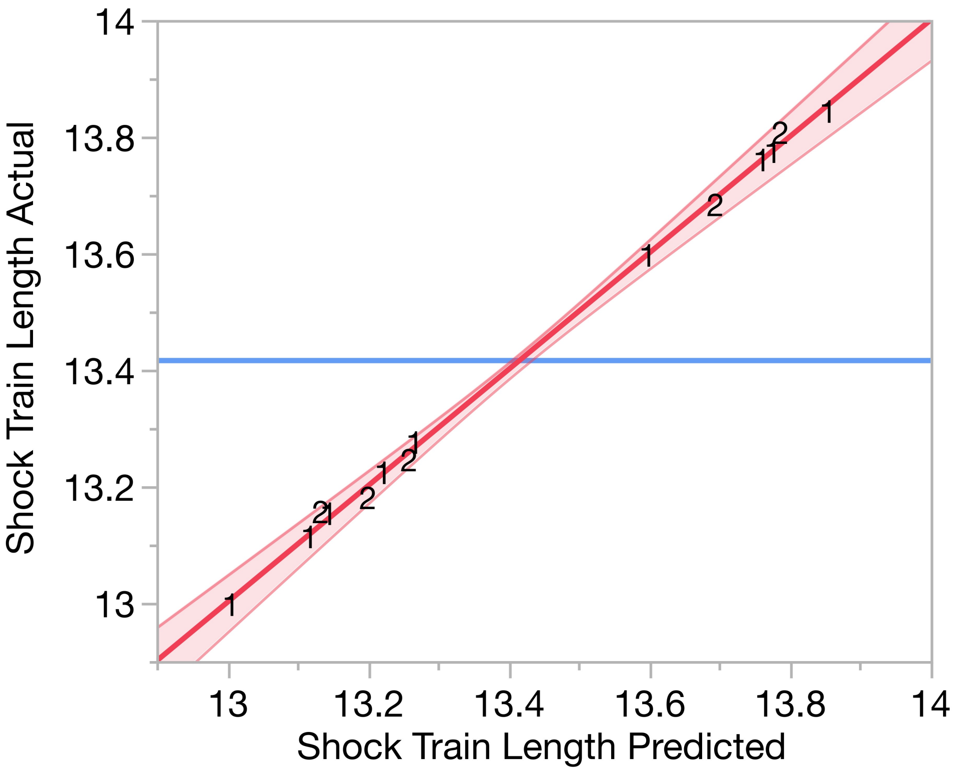
Shock Train Sensitivity to Back-Pressure

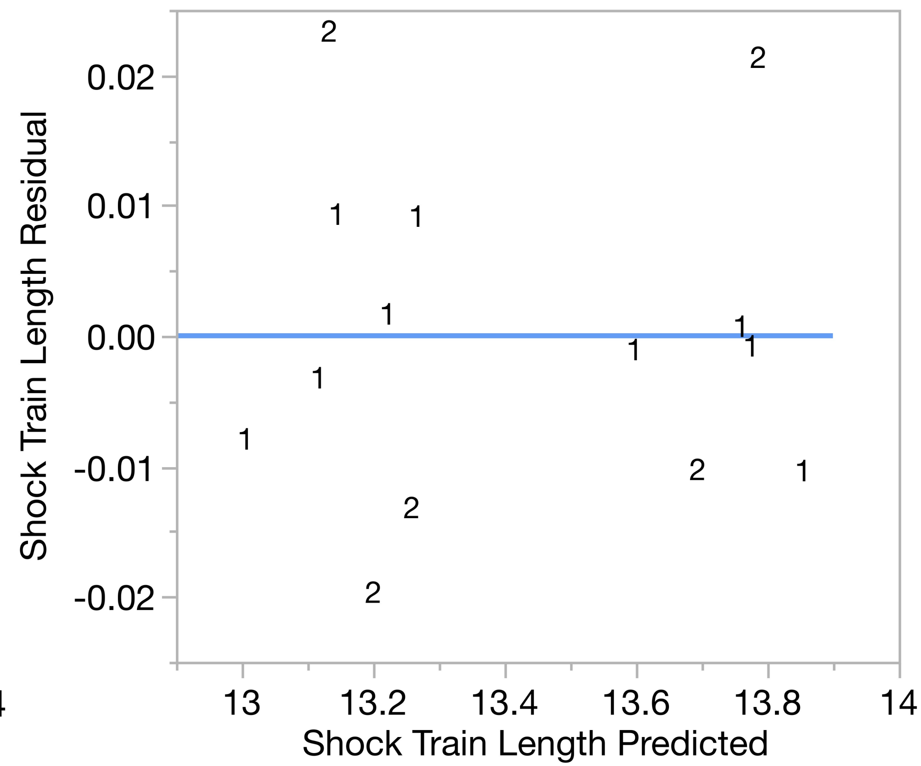


Metamodel Adequacy of Fit

R2$_{adjusted}$: 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).

$R^2_{predicted}$: 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 **R2$_{adjusted}$** to provide model stability confidence).





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