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A 2nd Order Uncertainty Quantification Framework Applied to a Turbulence Model Validation Effort

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Assessing the Credibility of CFD Results



- **Scramjet engine 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 hindered by harsh scramjet flow environment
  - 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

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

- **UQ approach of Roy et al. (AIAA Paper 2010-0124)**
  - Approach is a 2nd-order approach to uncertainty quantification
    - Aleatory and Epistemic uncertainty sources treated differently
  - Aleatory uncertainties are typically irreducible and inherently random, and as a result described by PDFs.
  - Epistemic uncertainties are systematic uncertainties that result from inadequate knowledge … these sources of uncertainty are reducible if further knowledge is gained.

Uncertainty Quantification Framework

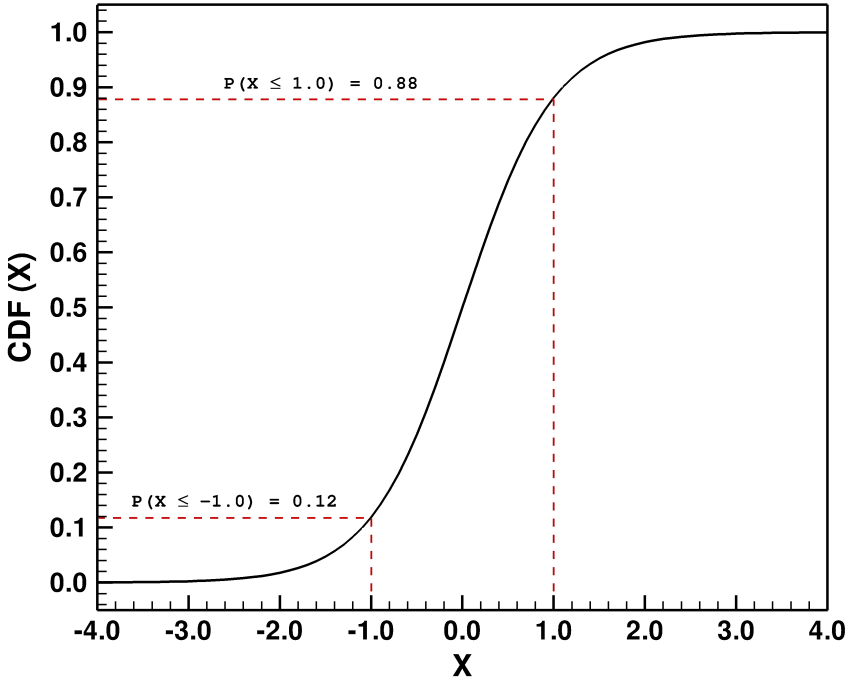
Steps in the UQ process:

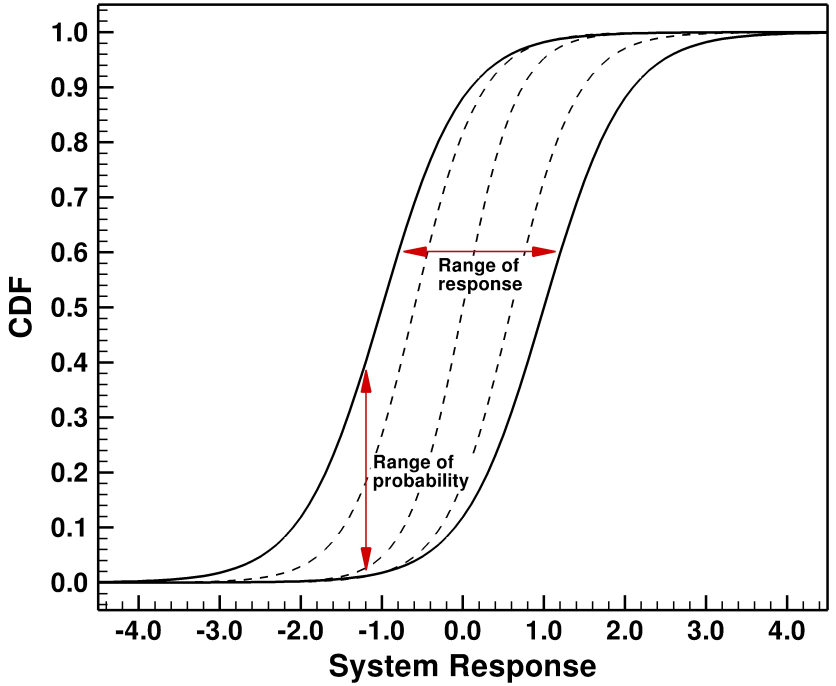
(1) Identify and characterize each uncertainty

(2) Prioritize the sources of uncertainty

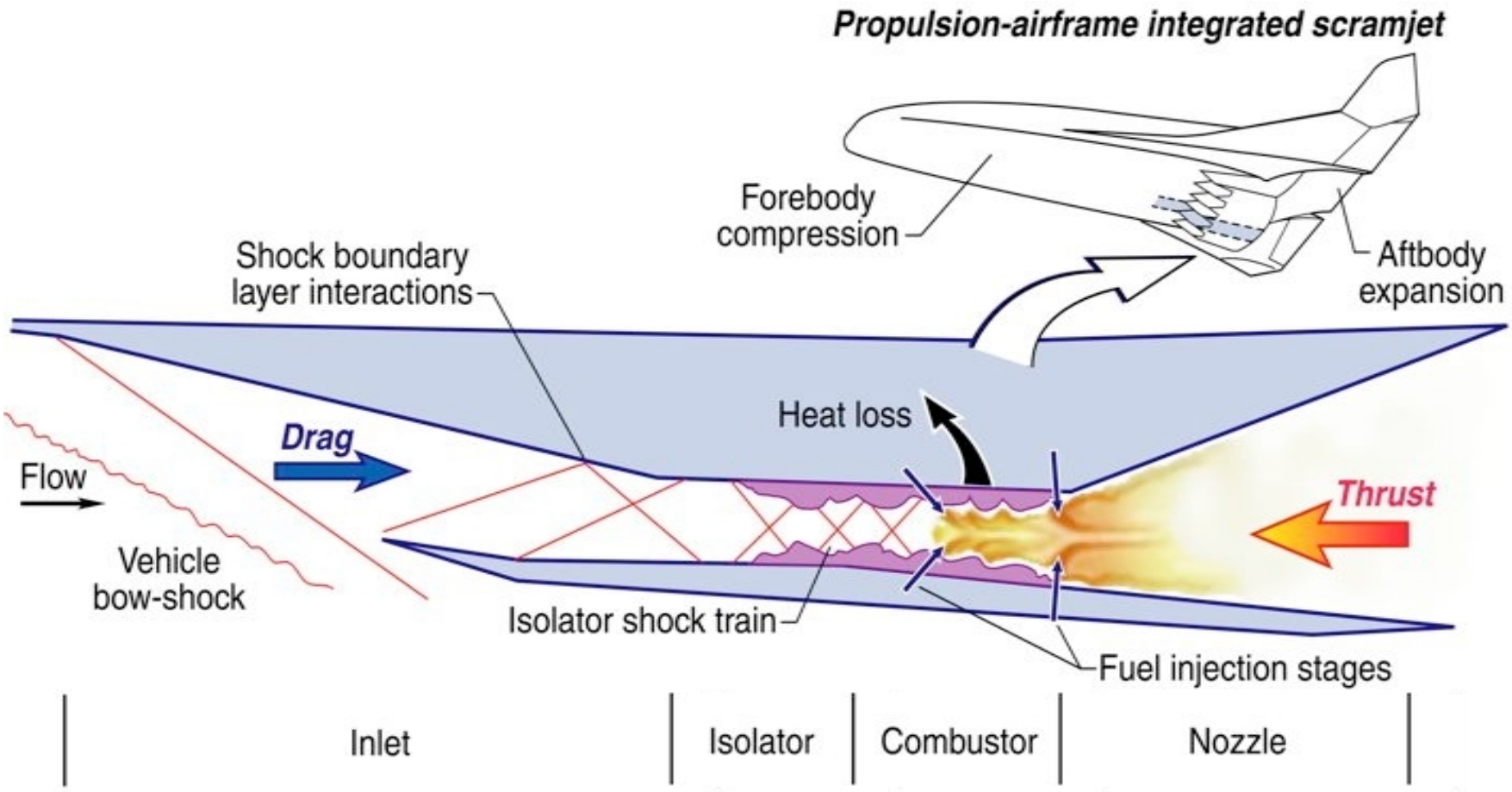
(3) Propagate the uncertainties through the "computational model" to extract the QoI

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

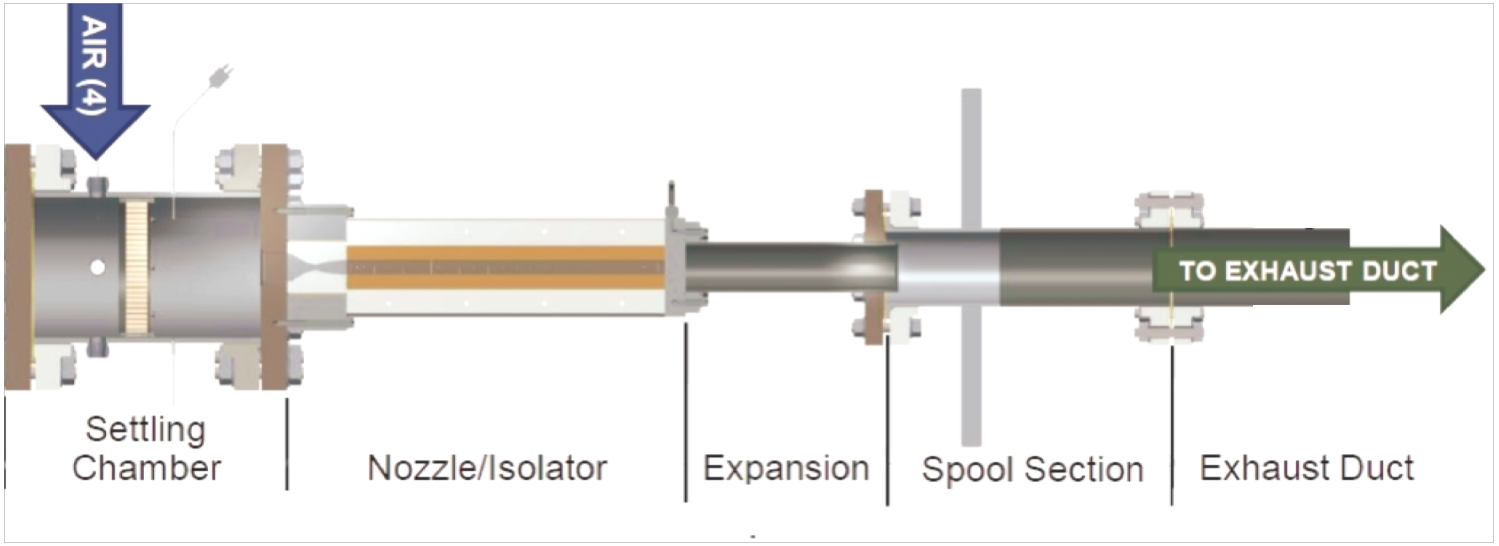




Scramjet Engine Flow Features …



IDRL Facility Description and Conditions

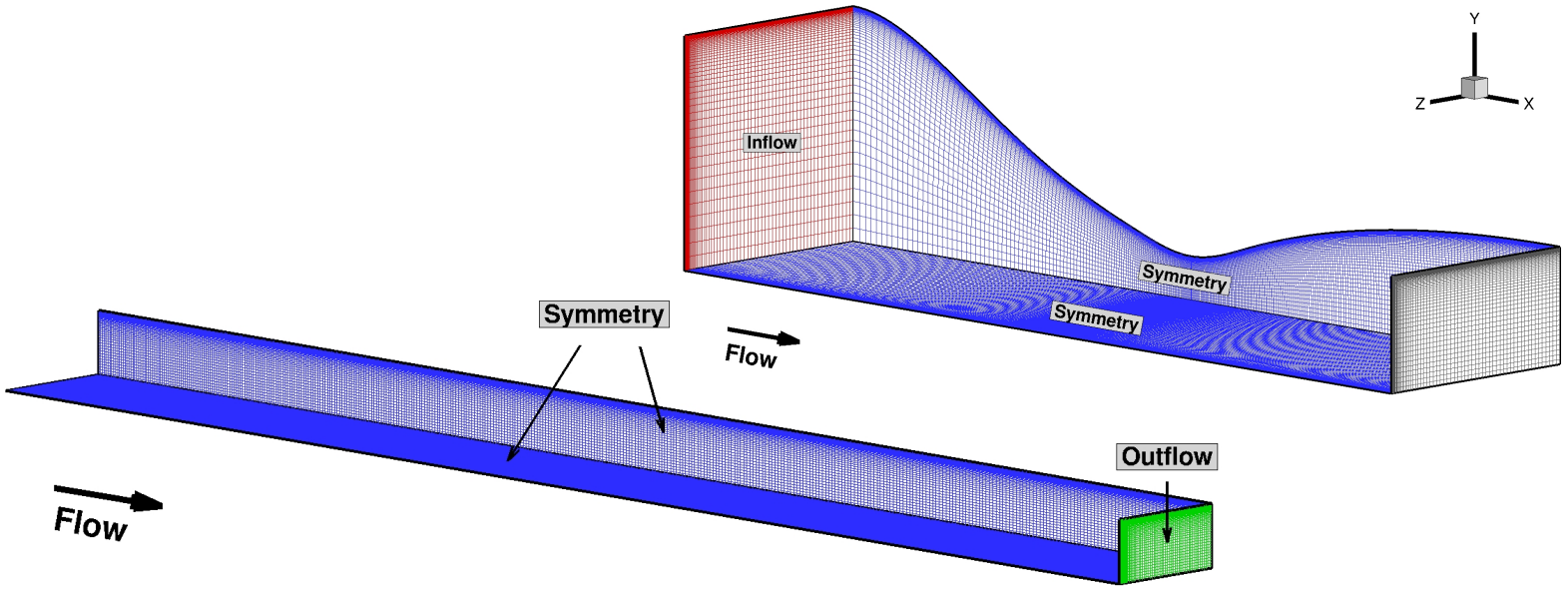


Facility Property	Operating Condition
Nozzle Plenum Pressure [kPa]	908.7* (0.027)
Nozzle Plenum Temperature [K]	292.9 (0.023)
Nozzle Exit Mach Number	2.5*
Nozzle Exit Pressure [kPa]	53.9
Isolator Exit Pressure [kPa]	311.6 (0.097)

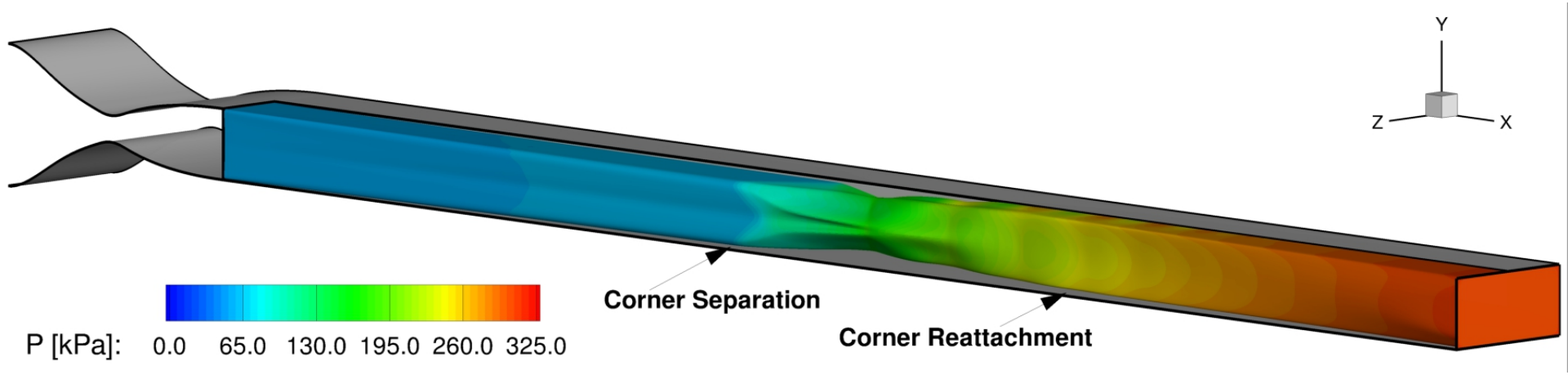
* Nominal value from isentropic relationships

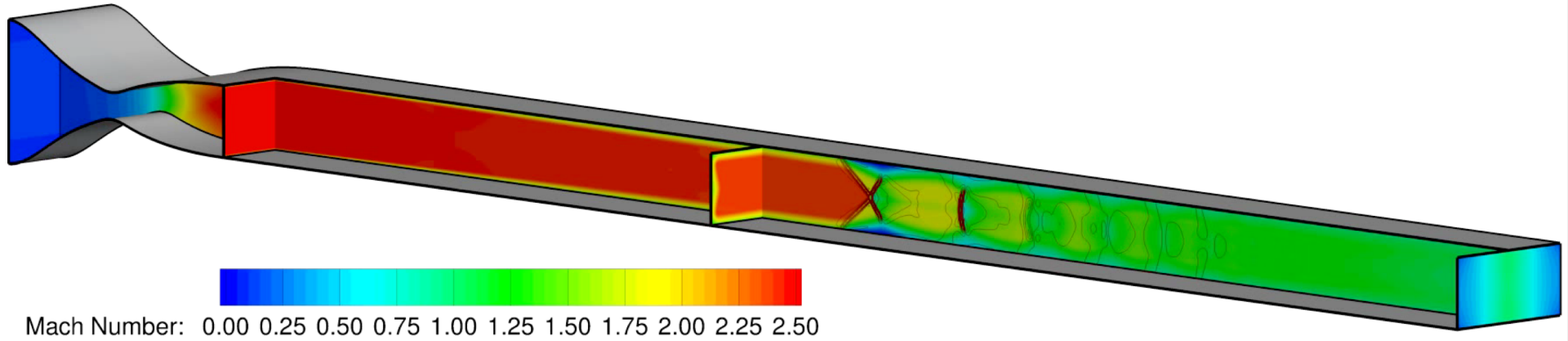
Simulation Description

- **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)

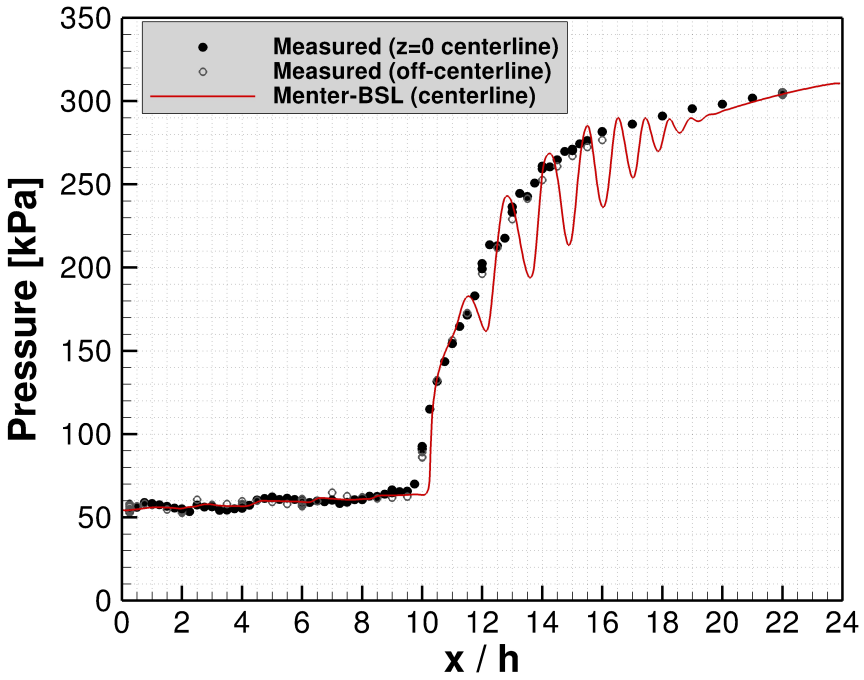


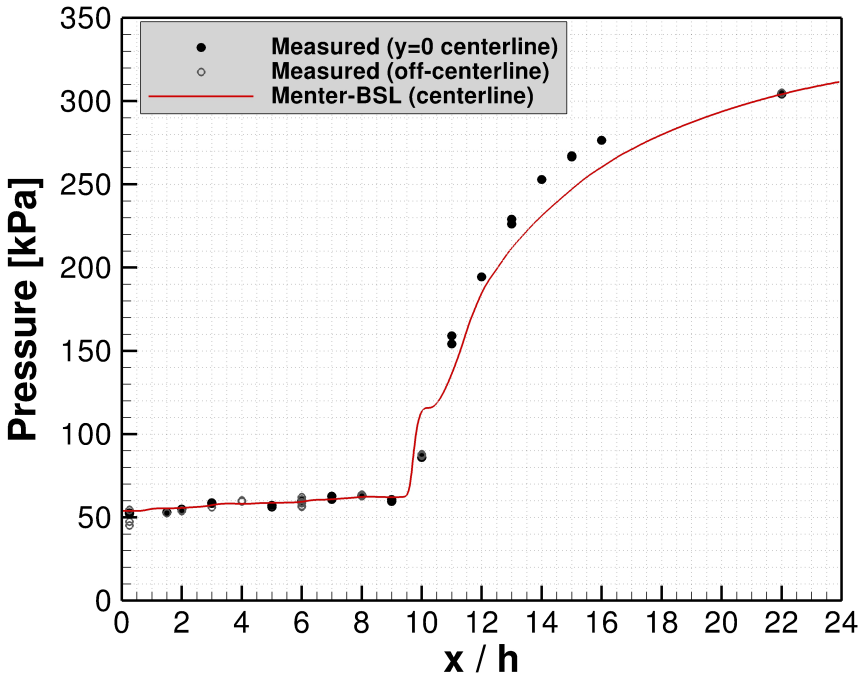
Isolator Flowfield Description





Nominal Comparison with Measurements





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



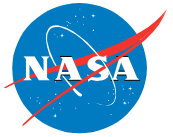
- **Step 1: Identify and characterize potentially important uncertainty sources**
  - Spatial discretization error (EPISTEMIC)
  - Onset of laminar to turbulent transition (EPISTEMIC)
  - Facility supply pressure (ALEATORIC)
  - Facility supply temperature (ALEATORIC)
  - Facility supply turb. intensity (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



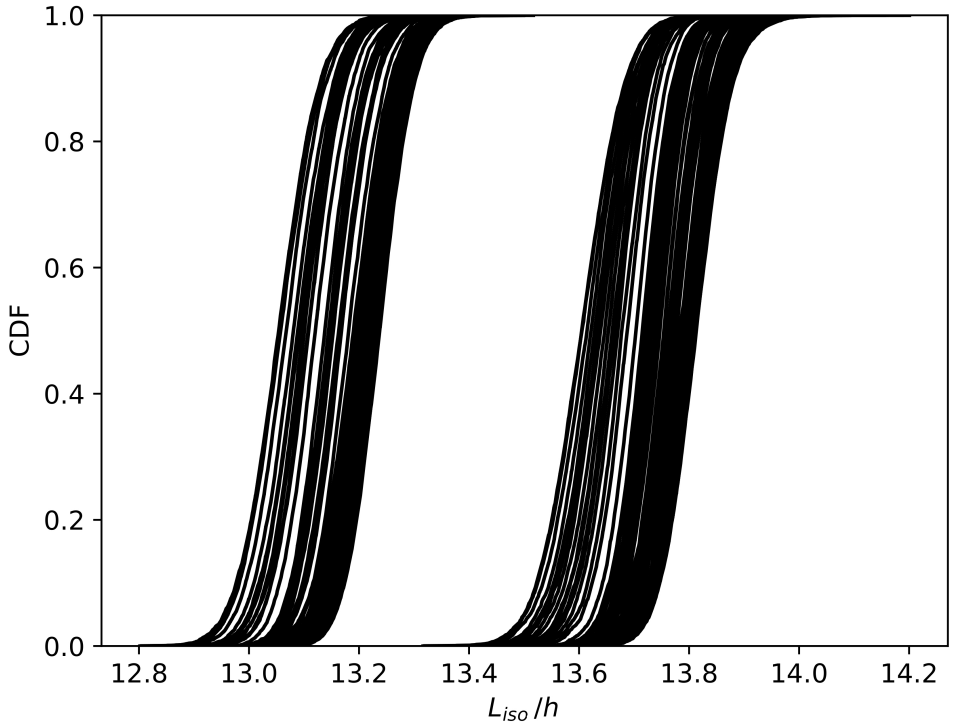
- **Step 3a: Build a metamodel for QoI for the uncertainty propagation**
  - Key cost-saving step since the direct use of 3-D CFD for uncertainty propagation would be impractical.
  - Design space used to construct the metamodel based on bounding estimates of each uncertainty variable:
    - Facility 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, N_e
  Do m = 1, N_a
    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)

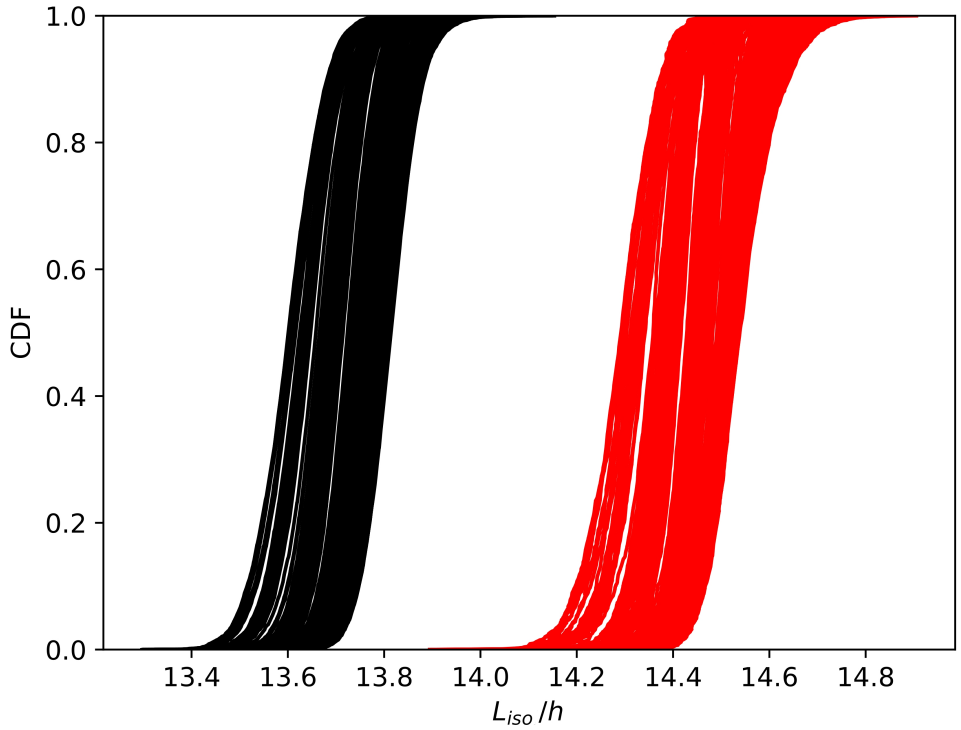


Validation with Uncertainty

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

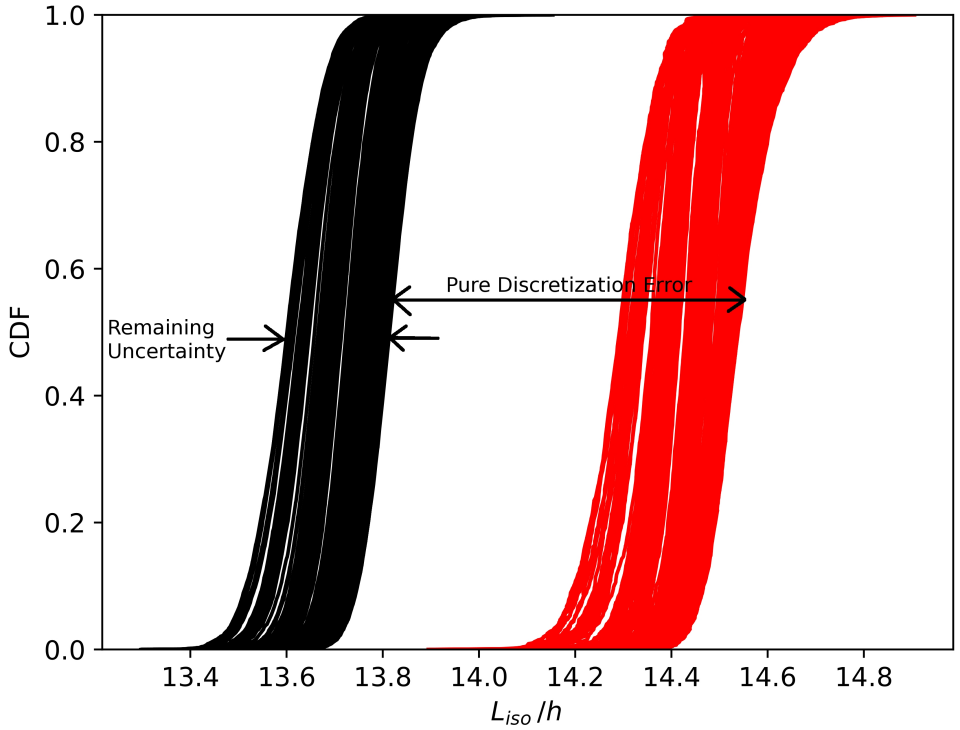
$$\mathrm{GCI} = F_s \frac{|f_2 - f_1|}{r^p - 1}$$

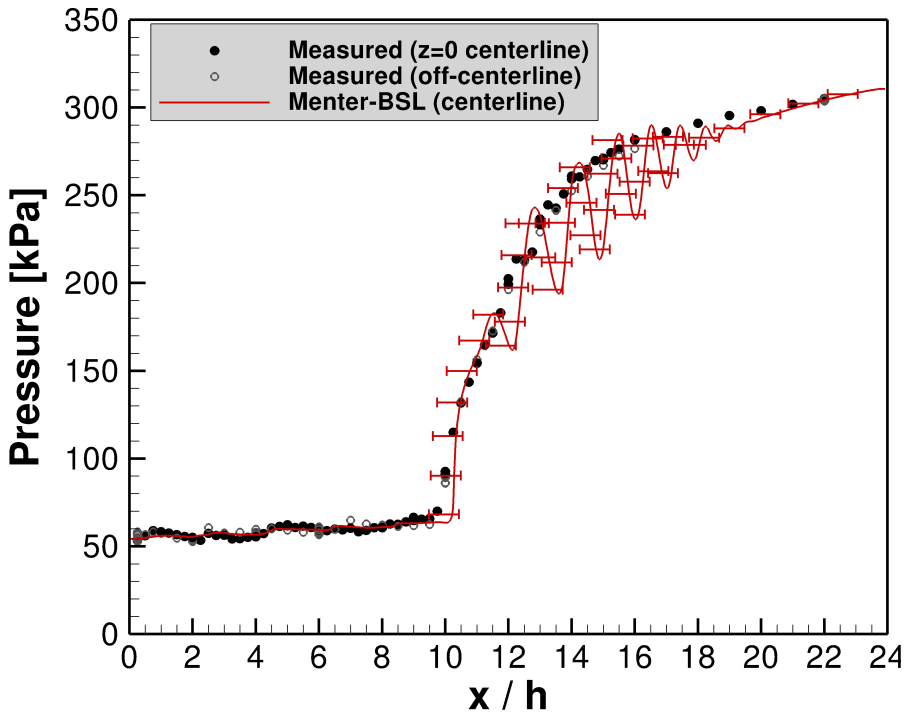
$$\mathrm{L}_{iso^*} - \mathrm{L}_{iso^2} = F_s \frac{\mathrm{L}_{iso^2} - \mathrm{L}_{iso^1}}{r^p - 1}$$



Validation with Uncertainty

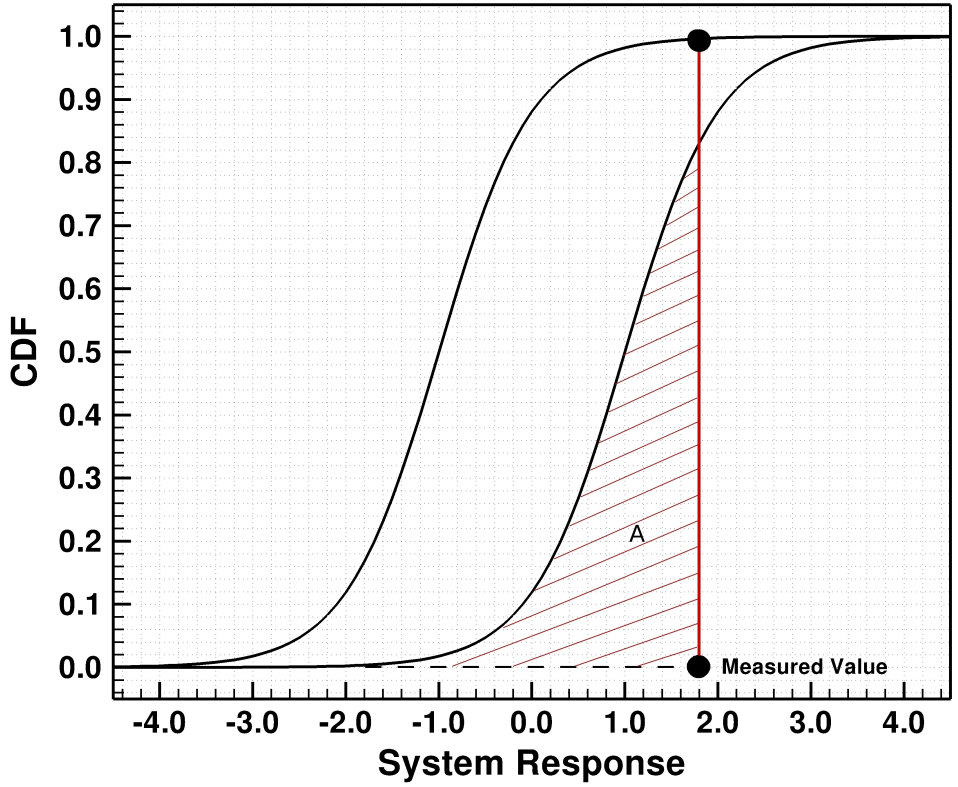
- **The UQ information can also be displayed in a more conventional manner as error bars.**
  - Discretization error is known to be a one-sided bias error
  - Remaining error is equally distributed on the uncertainty bar

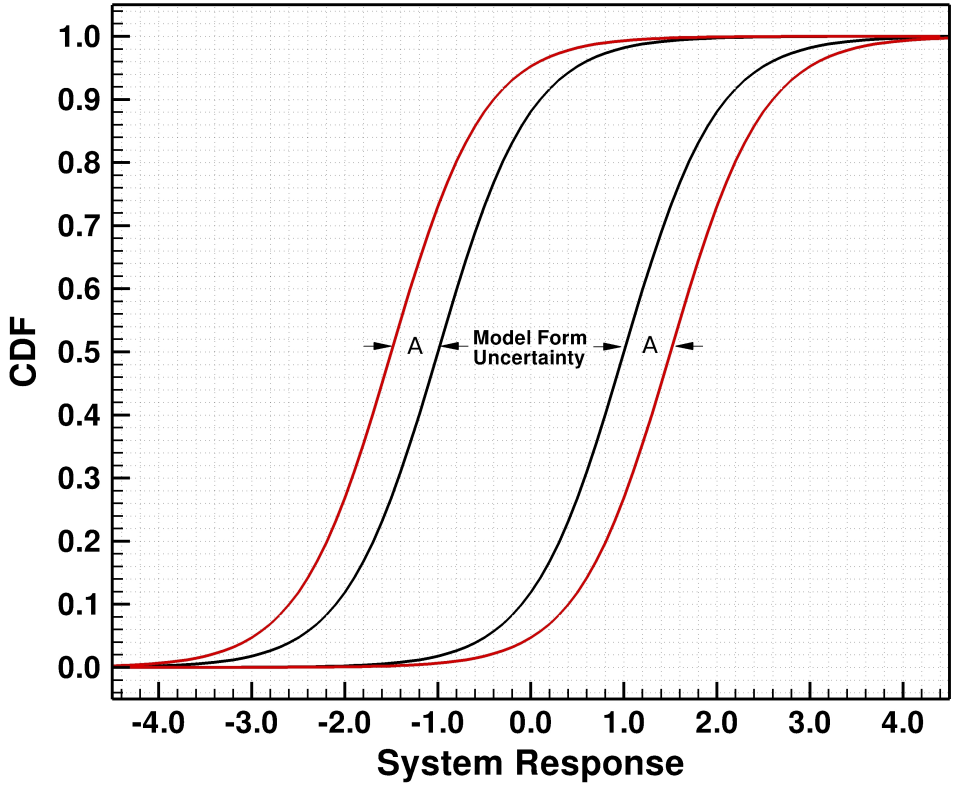




Determination of Model-Form Uncertainty

- **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
  - Largest area validation metric used to pad the Probability-Box



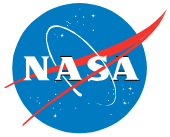


Summary

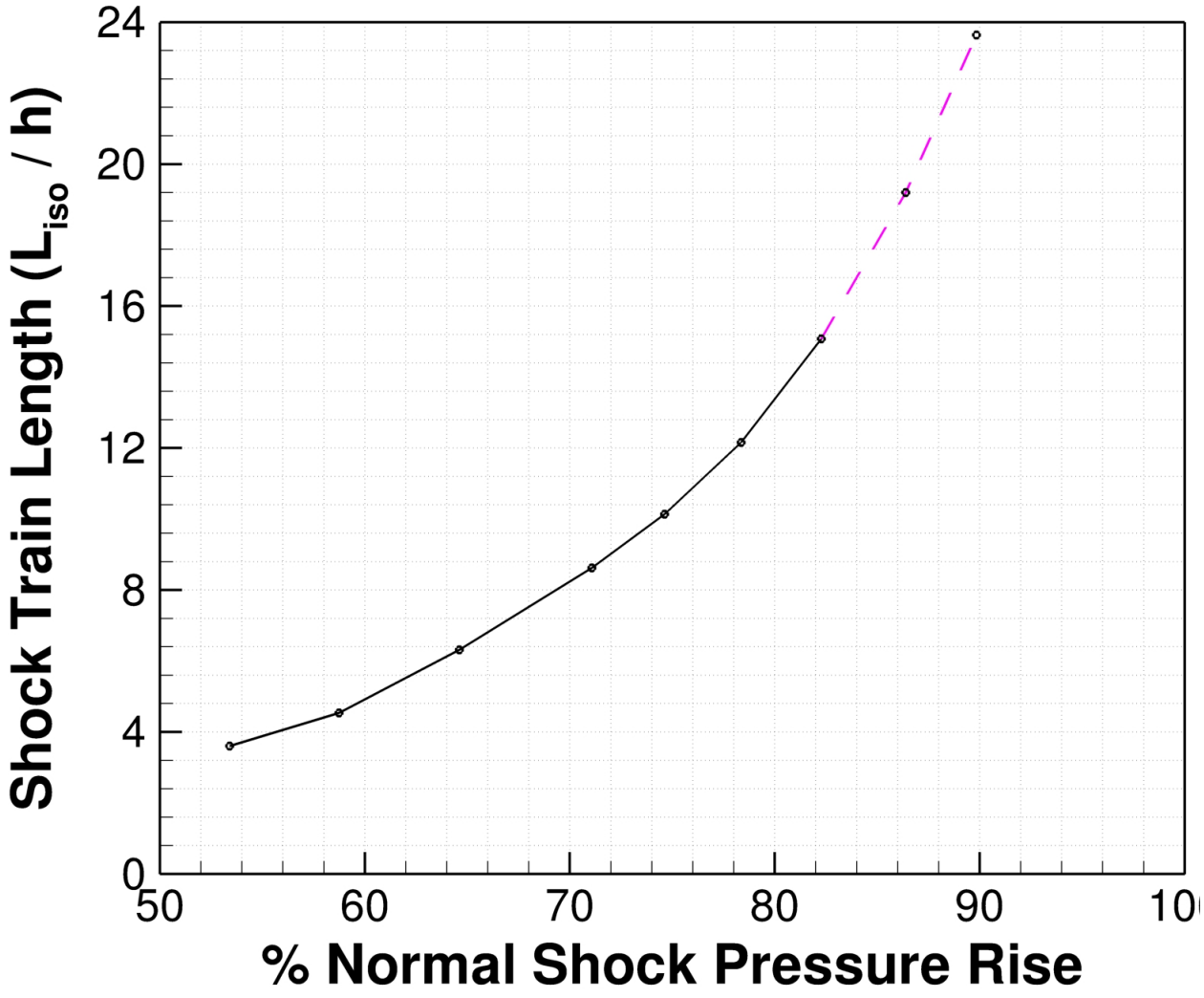


- **High-fidelity CFD data plays a dominant role in the design/analysis of aerospace vehicles.**
  - Continual desire to rely more on CFD and less on ground testing.
- **A UQ-centric approach to CFD has been demonstrated to provide "Risk Informed" decisions.**
  - Confidence in simulation data needs 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 utilized in the context of a CFD validation process.**
- **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 …



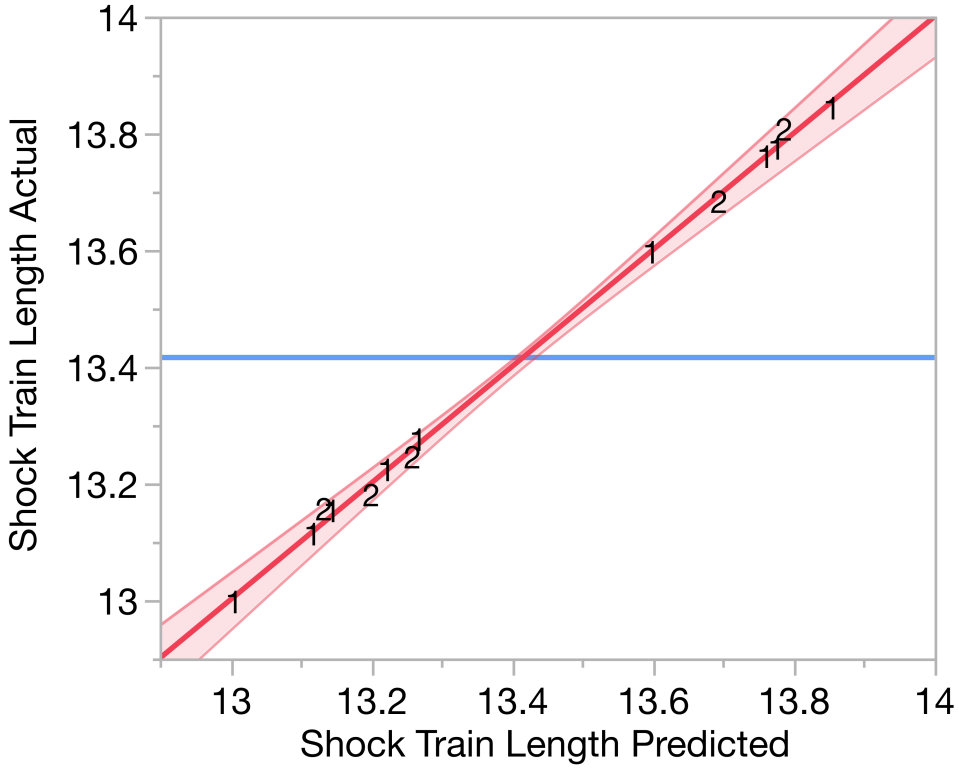
Shock Train Sensitivity to Back-Pressure

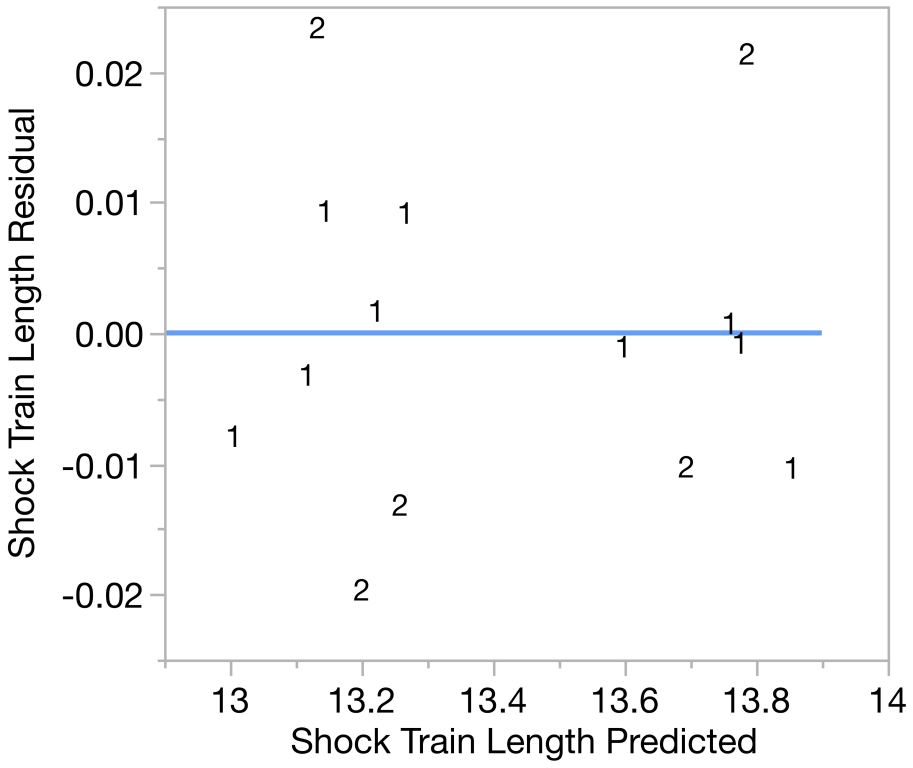


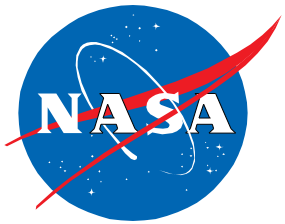
Metamodel Adequacy of Fit

$R2_{adjusted}$: 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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