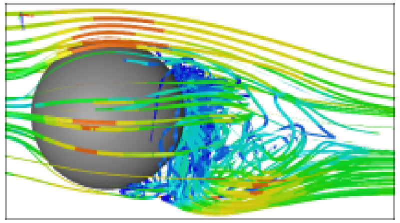
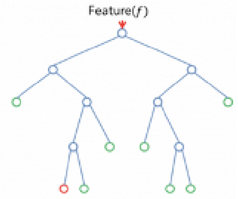
APS DFD 2024, Nov 24-26, Salt Lake City

SAND2024-15782C

Sandia National Laboratories

Robust Data-Driven Turbulence Modeling for RANS Closures Using a SciML Approach for Validation





PRESENTED BY: Uma Balakrishnan

Collaborators: William J Rider, Matthew Barone, Eric J. Parish

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VERIFICATION VALIDATION

U.S. DEPARTMENT OF ENERGY NNSA

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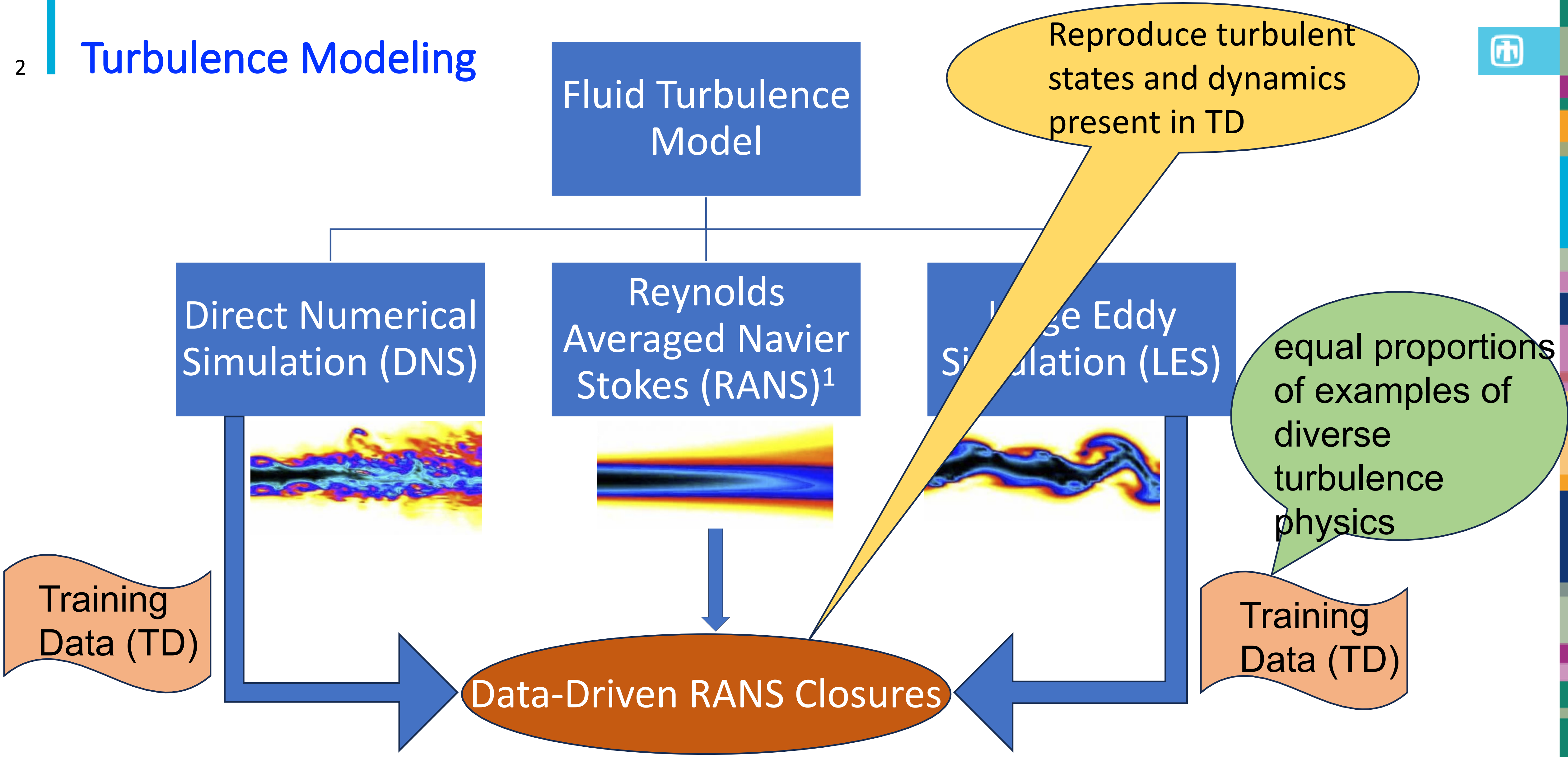
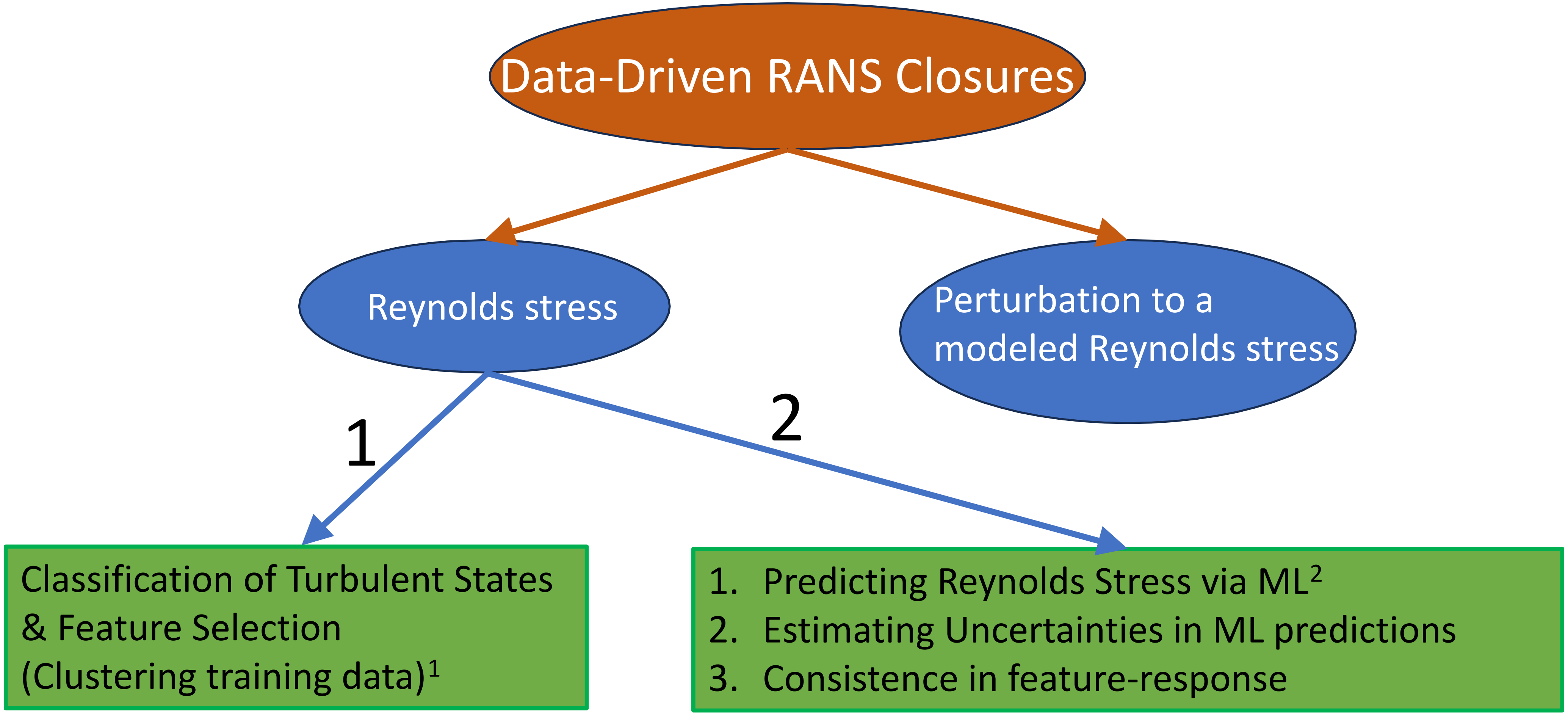
Turbulence Modeling



1. J. Ling, J. Templeton, and A. Kurzawski, Reynolds averaged turbulence modelling using deep neural networks with embedded invariance, JFM, Vol 807, 2016, 155-166.

Data-Driven Turbulence Modeling



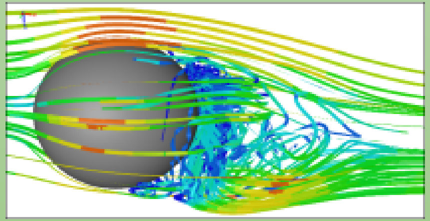
1. M.F.Barone, J.Ray, and S.Domino, Feature Selection, Clustering, and Prototype Placement for Turbulence Datasets , AIAA Journal 2022 60:3, 1332-1346.

2. E. Parish, D.S. Ching, N.E. Miller, S. J. Beresh and M. F. Barone. "Turbulence modeling for compressible flows using discrepancy tensor-basis neural networks and extrapolation detection," AIAA 2023-2126. *AIAA SCITECH 2023 Forum*. January 2023.

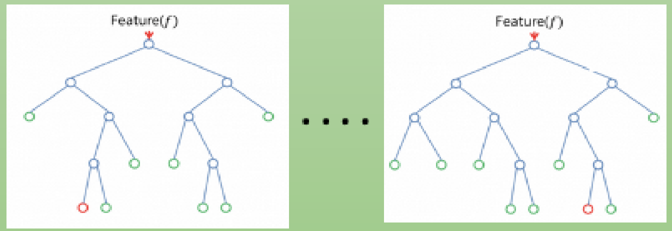
Motivating Credibility for Scientific Machine Learning (SciML)

Machine learned models are used in lieu of, complementary to, or as surrogates for science and engineering computational simulation models.

What does VV/UQ/Credibility Mean for Scientific Machine Learning?



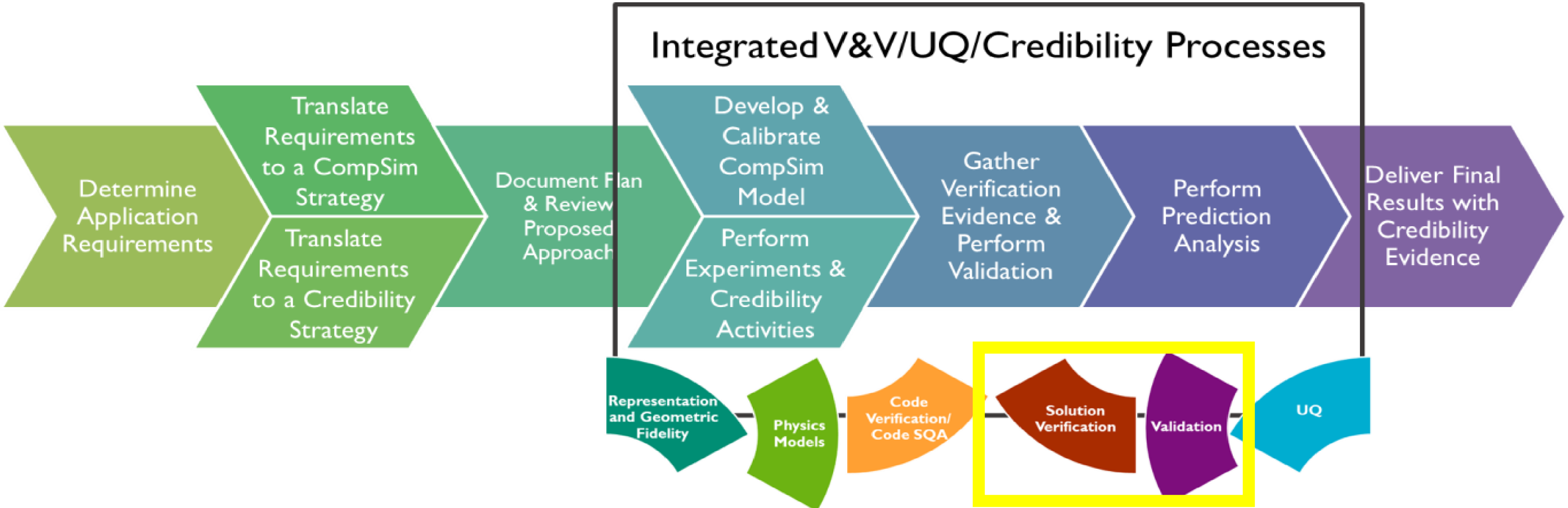
Scientific Computing



Machine Learning

Putting "correct" math methods and physics models into our codes.

Produce "correct" codes and models which leads to "correct" results.



Data-Driven Turbulence Modeling

$$a_{ij} \approx a_{ij}^{\mathrm{RANS}} + m_{ij}^{\mathrm{ML}}$$

Anisotropy-based discrepancy term

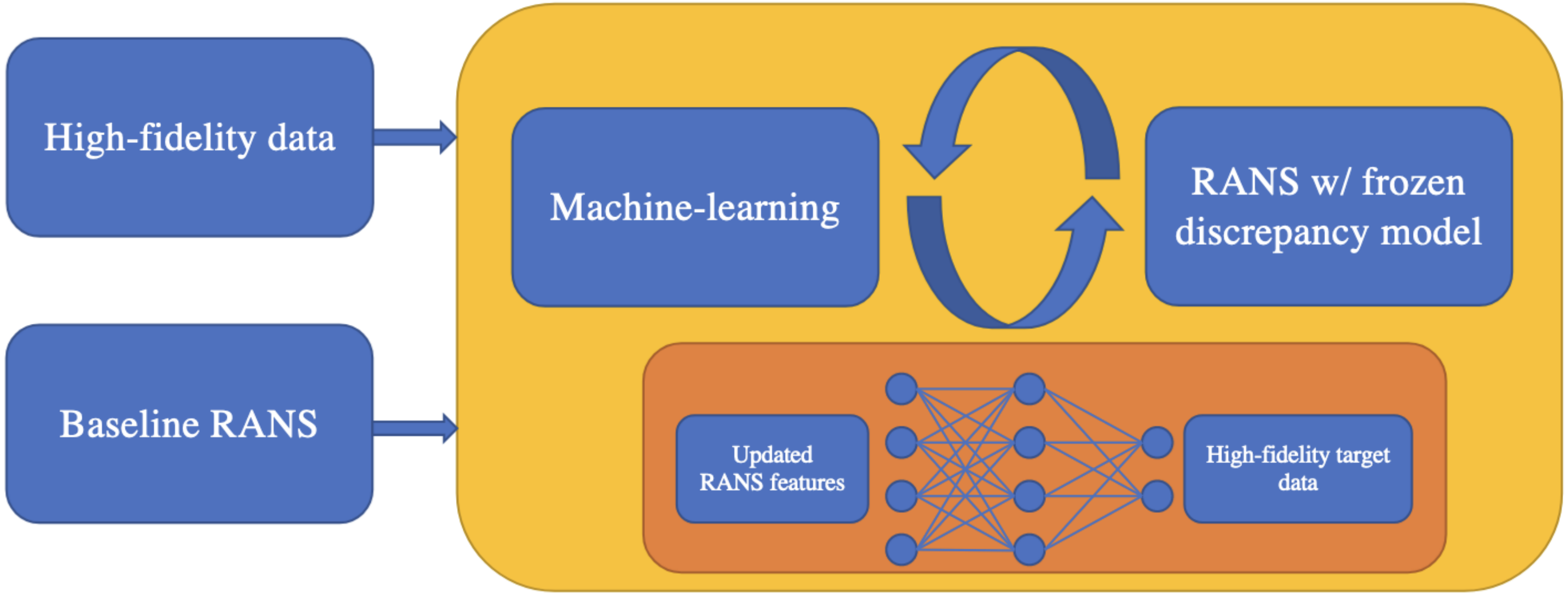
Anisotropy tensor

$$a_{ij} = \frac{-\tau_{ij}}{\overline{\rho u_k'' u_k''}} - \frac{1}{3}\delta_{ij}$$

Anisotropy tensor predicted by a standard RANS

$$a_{ij}^{\mathrm{RANS}} = \frac{\tau_{ij}^{\mathrm{RANS}}}{2\bar{\rho}\tilde{k}} - \frac{1}{3}\delta_{ij}$$

δ_{ij} is the Kronecker delta & m_{ij}^{ML} is an ML correction



Iterative training procedure

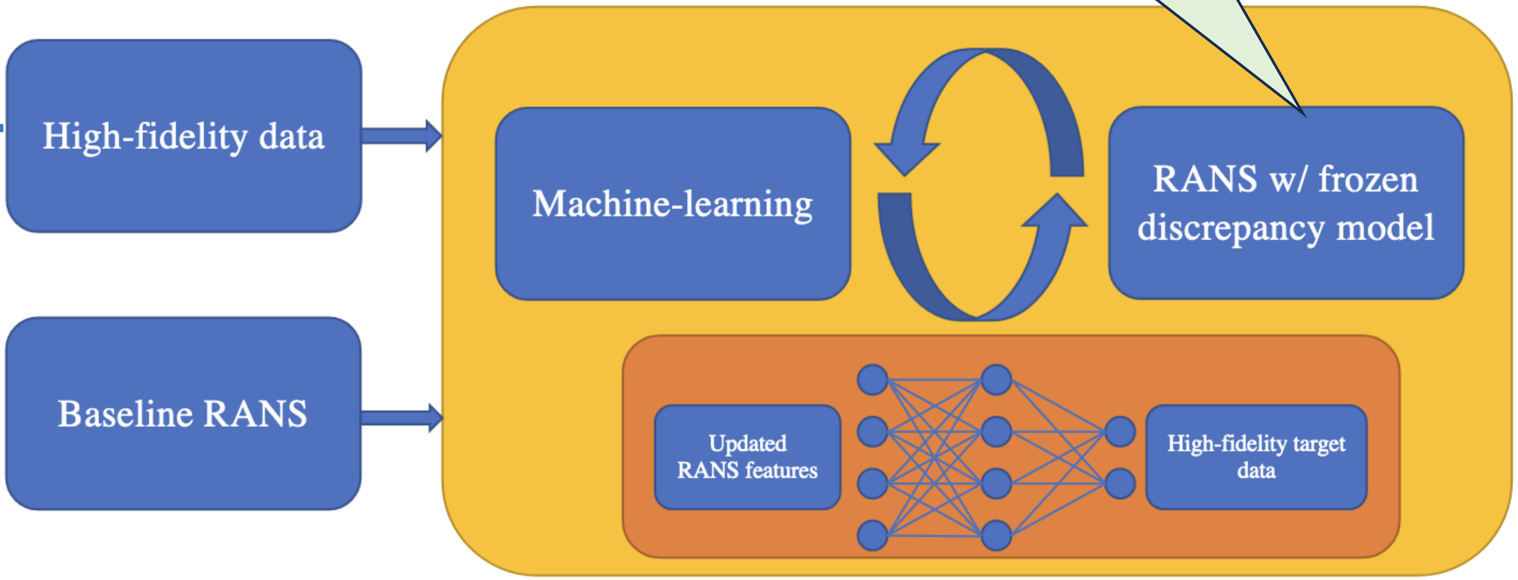
2. E. Parish, D.S. Ching, N.E. Miller, S. J. Beresh and M. F. Barone. "Turbulence modeling for compressible flows using discrepancy tensor-basis neural networks and extrapolation detection," AIAA 2023-2126. *AIAA SCITECH 2023 Forum*. January 2023.

Data-Driven Turbulence Modeling

$$a_{ij} \approx a_{ij}^{\text{RANS}} + m_{ij}^{\text{ML}}$$

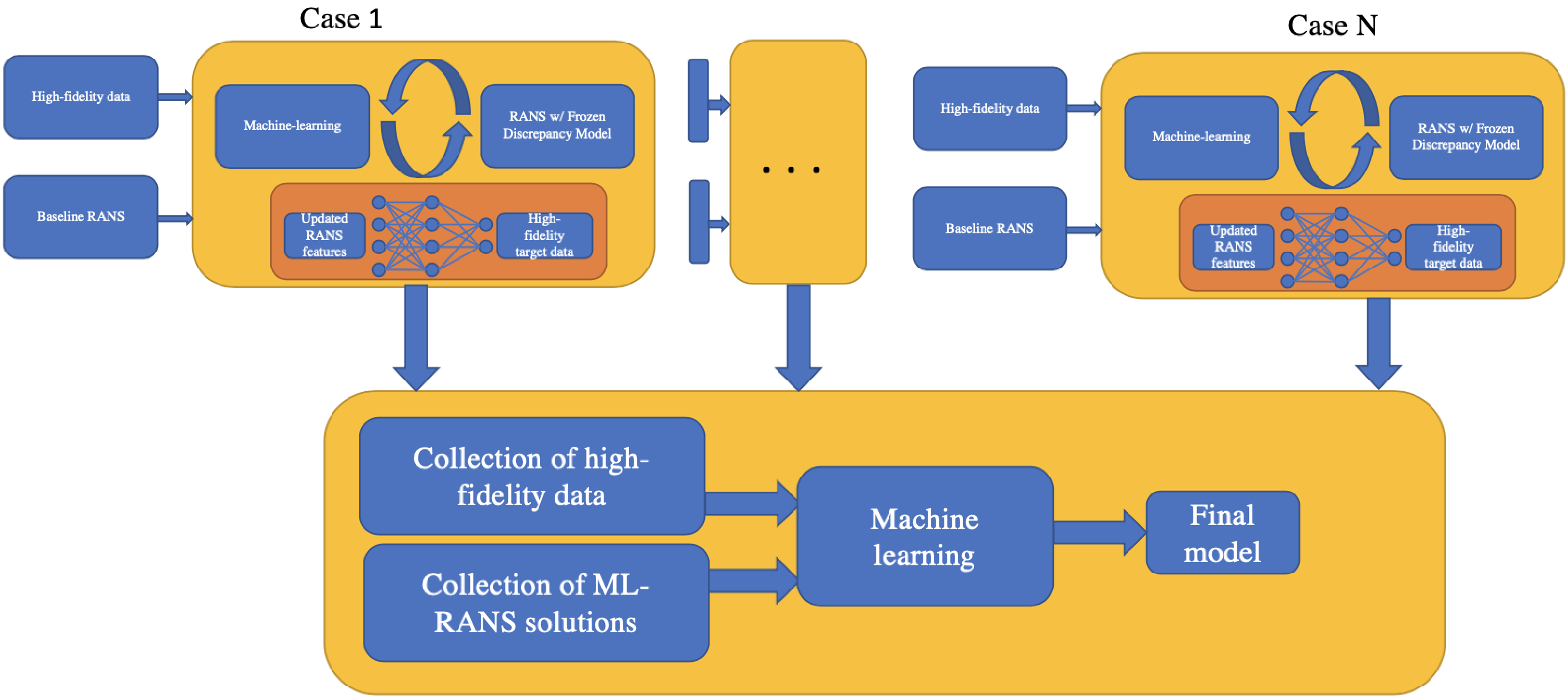
Discrepancy modes for an anisotropy tensor are implemented in Sandia's Parallel Aerodynamics Re-entry Code (SPARC) which supports various discretization

High Fidelity Datasets for Training
A. Channel flow with Re = 180
B. Channel flow with Re = 395
C. Channel flow with Re = 590
D. Duct flow at Re = 3500
E. Flow over periodic hill
F. HS BL at M = 6, $T_w/T_r = 0.25$
G. HS BL at M = 6, $T_w/T_r = 0.76$
H. HS BL at M = 14, $T_w/T_r = 0.18$



2. E. Parish, D.S. Ching, N.E. Miller, S. J. Beresh and M. F. Barone. "Turbulence modeling for compressible flows using discrepancy tensor-basis neural networks and extrapolation detection," AIAA 2023-2126. *AIAA SCITECH 2023 Forum*. January 2023.

Global Training Process



Data-Driven Turbulence Modeling

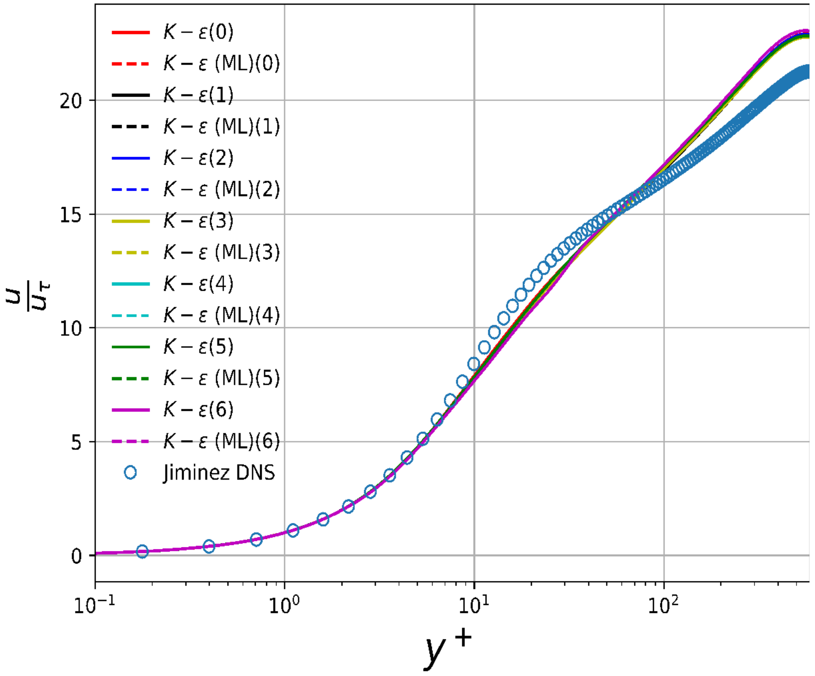
- Global iterative training procedure improves feature consistency.
- Complete consistency in response has not been achieved.
- The goal is to minimize overall inconsistency.
- ML models involve many hyperparameters.
- Considering various combinations of training datasets and testing hyperparameters might help validate and improve the overall response consistency.

Various Combination of Training Datasets

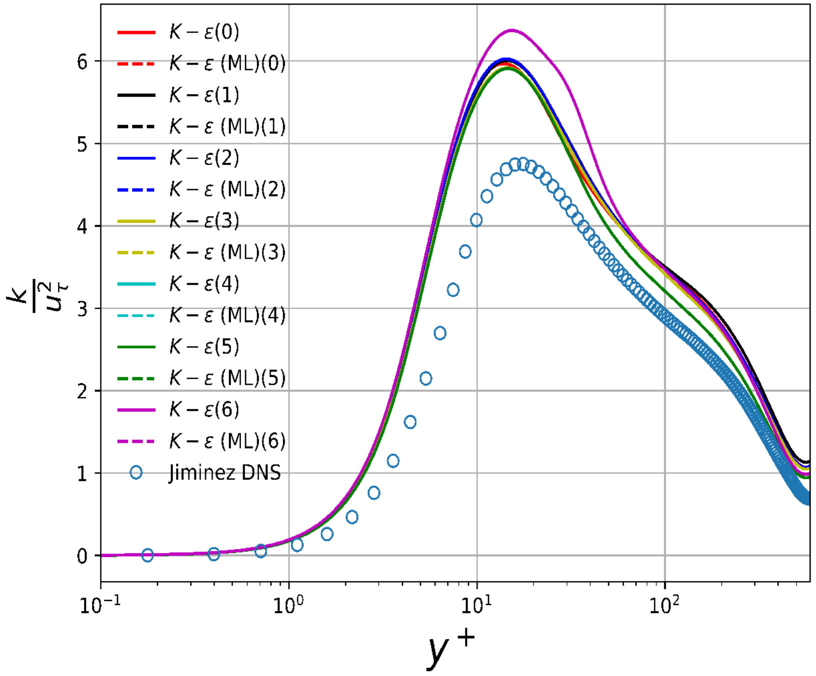
High Fidelity Datasets for Training
A. Channel flow with Re = 180
B. Channel flow with Re = 395
C. Channel flow with Re = 590
D. Duct flow at Re = 3500
E. Flow over periodic hill
F. HS BL at M = 6, $T_w/T_r = 0.25$
G. HS BL at M = 6, $T_w/T_r = 0.76$
H. HS BL at M = 14, $T_w/T_r = 0.18$

Combination of Datasets
(0) A, B, C, D, E, F, G, H
(1) B, C, D, E, F, G, H
(2) A, C, D, E, F, G, H
(3) A, B, D, E, F, G, H
(4) A, B, C, D, E, G, H
(5) A, B, C, D, E, F, G
(6) A, B, C, D, E, F, H

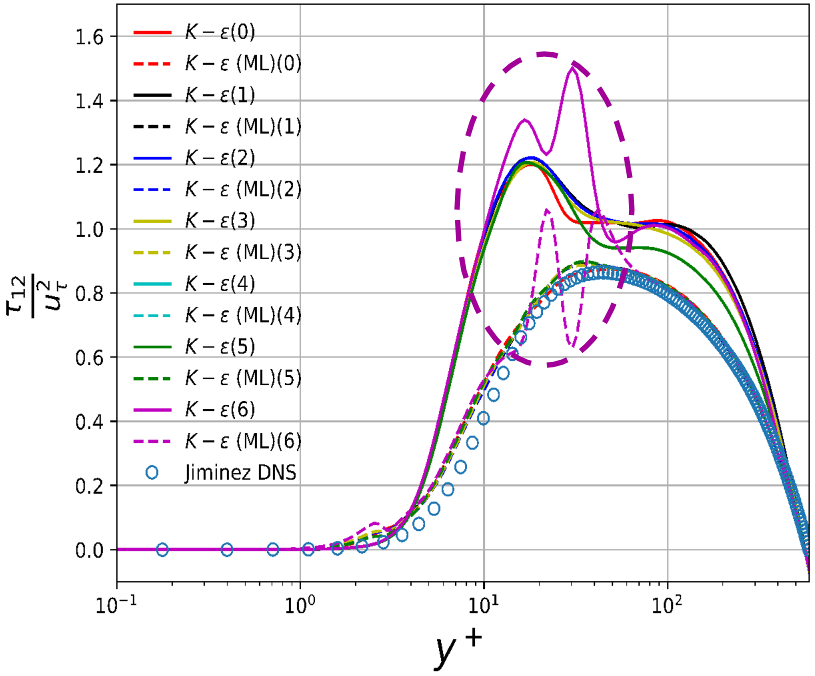
Validating Training Datasets & Testing Channel Flow



Velocity



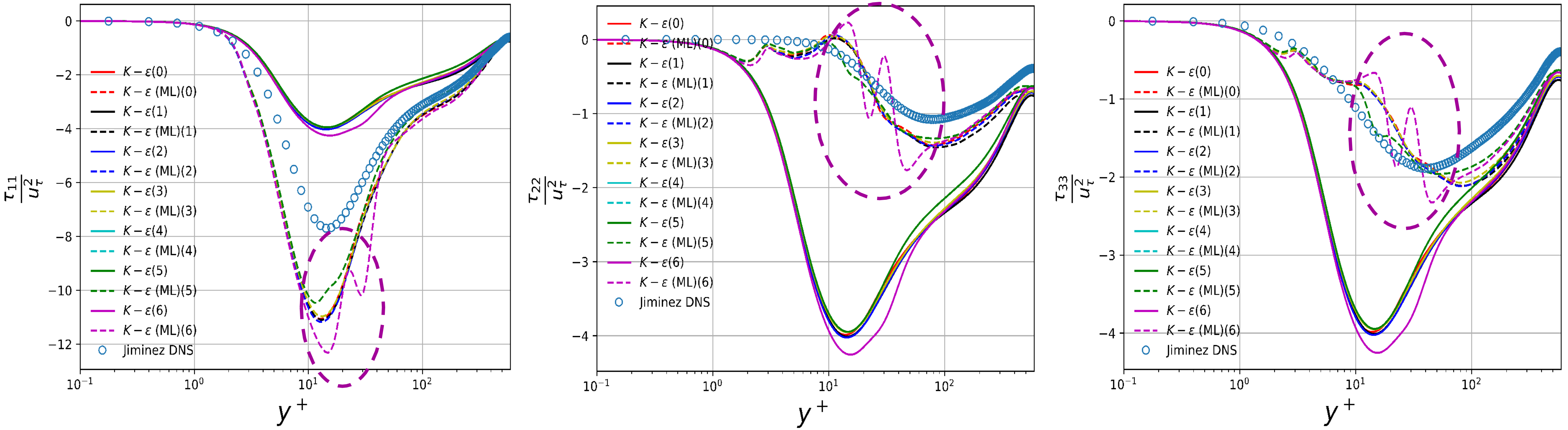
Turbulence Kinetic Energy



Reynolds Shear Stress

- ➢ The global iterative procedure was trained on various combinations of datasets as described in the previous slide (w/o changing any hyperparameters).
- ➢ It was then tested on the channel flow dataset with Re = 590.

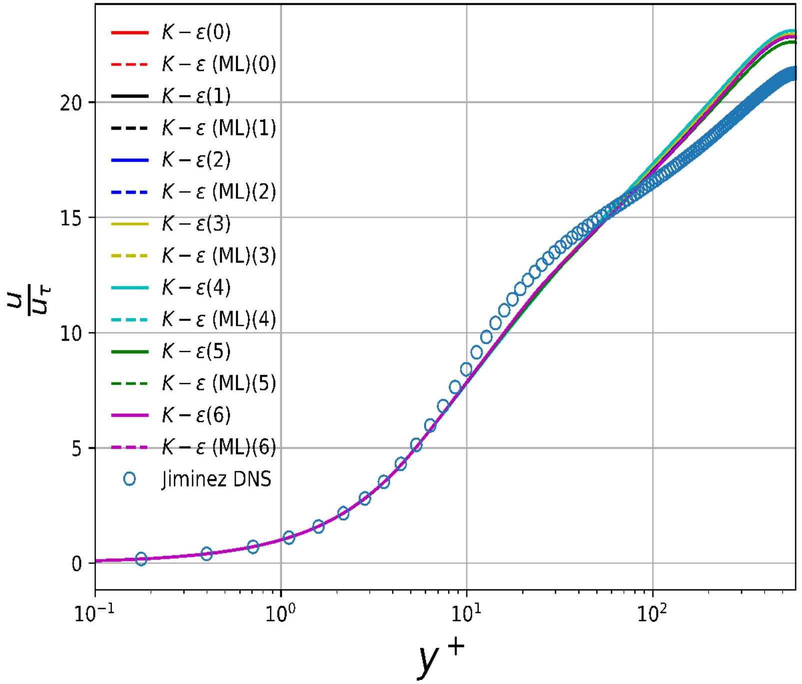
Validating Training Datasets & Testing Channel Flow



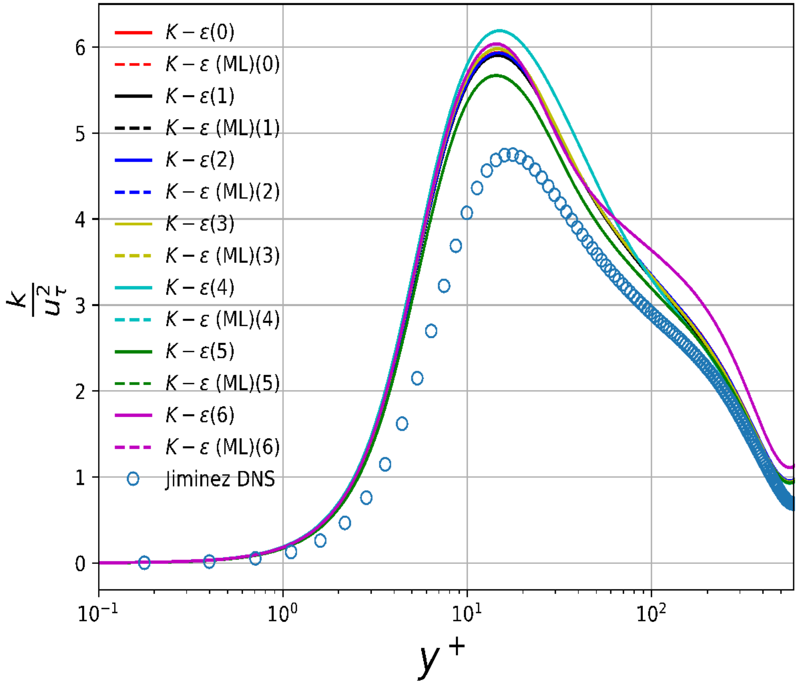
Normal Stress in x, y & z direction

- Figures clearly show that the ML correction term follows the trend of the "true" (DNS) data. However, there is a deviation in the buffer layer, which is consistent across all combinations of training datasets.
- Dataset combination (6) exhibits clear oscillations.

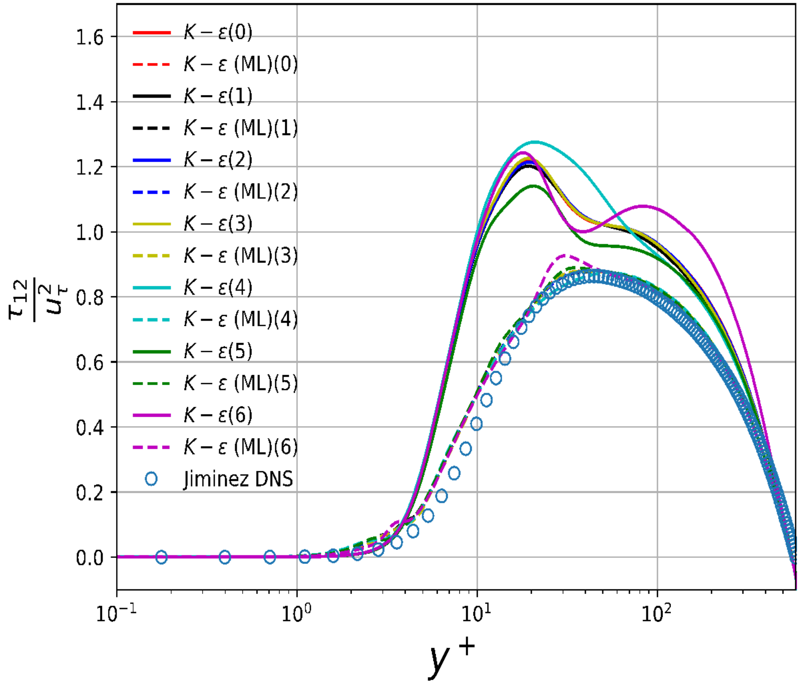
Validating Training Datasets & Testing Channel Flow



Velocity



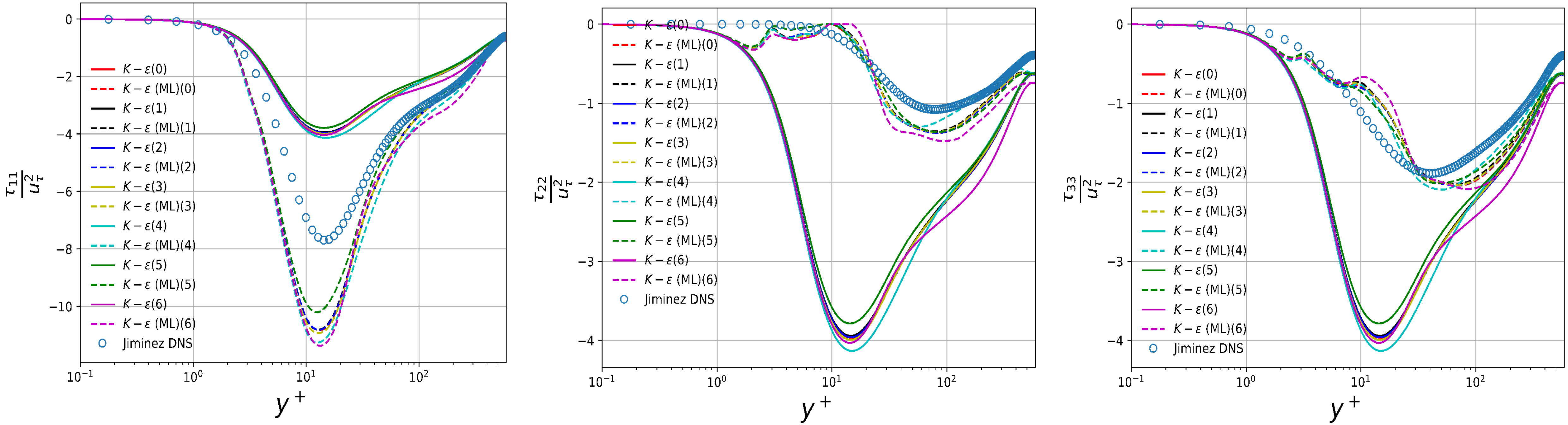
Turbulence Kinetic Energy



Reynolds Shear Stress

- ➢ Reducing the depth and width of the neural network along with an optimum epochs clearly reduces the overfitting problem.

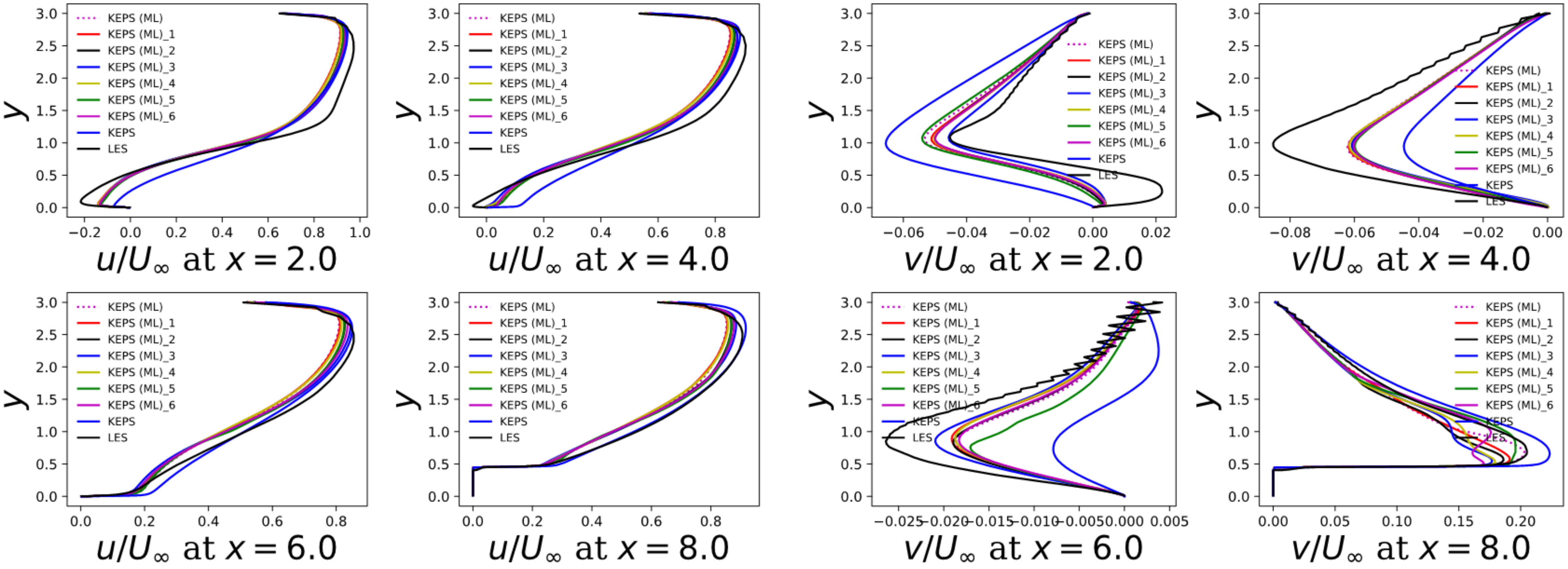
Validating Training Datasets & Testing Channel Flow



Normal Stress in x, y & z direction

- ➢ Reducing the depth and width of the neural network along with an optimum epochs clearly reduces the oscillatory behavior.
- ➢ However, there is still a deviation in the buffer layer, which is consistent across all combinations of training datasets.

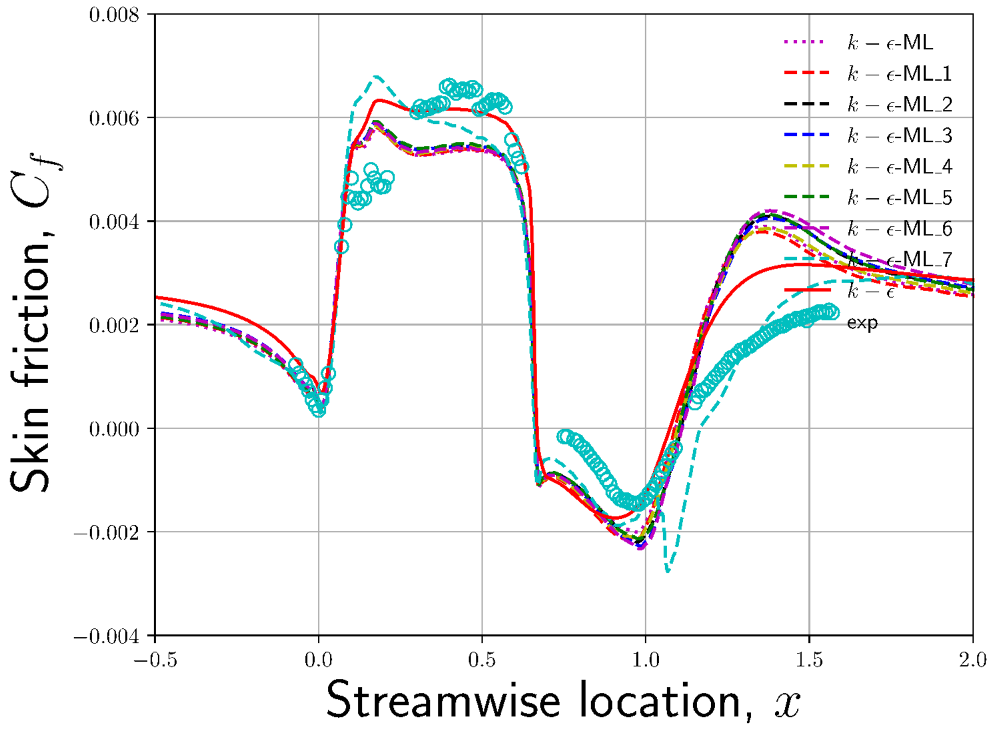
Validating Training Datasets & Testing Periodic Hill



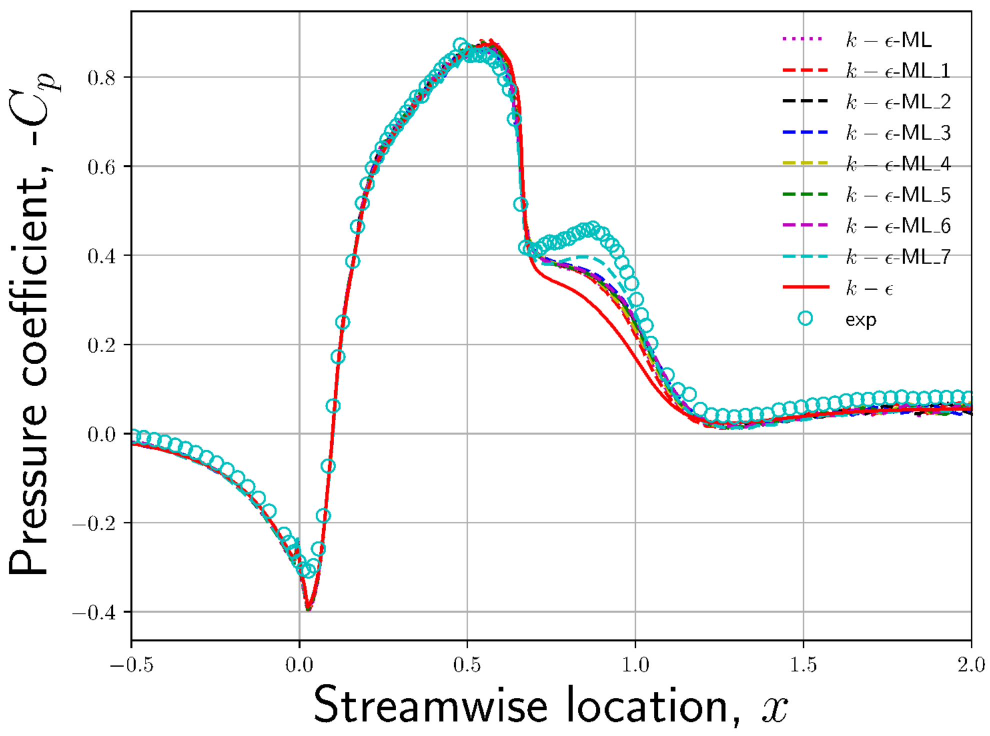
- ➢ We then tested on the Periodic Hill, and the figure shows the velocity profiles as a function of y for various x locations.

- ➢ The figures clearly show that the ML correction term performs better than the standard k–ϵ model.

Validating Training Datasets & Testing NASA Hump (Out-Of-Distribution)



Pressure Coefficient



Friction Coefficient

- Figure depicts the pressure coefficient and skin friction as a function of the streamwise location for the k–ϵ and k–ϵ–ML models.
- We observe that the k−ϵ−ML slightly under predicts the peak in pressure and friction coefficient which needs to be improved.

Conclusions and Future Work

- **Performance Consistency**: We conducted rigorous testing on a variety of in-distribution and out-of-distribution datasets using different combinations of training datasets, which demonstrated consistent performance across these combinations.

- **Hyperparameter Tuning**: Some combinations of training datasets highlight the need for hyperparameter tuning to reduce inconsistency in the anisotropy-based discrepancy term.

- **Network Depth Reduction**: Reducing the depth and width of the network effectively along with optimum epochs mitigates oscillation and overfitting, yet there remains inconsistent behavior in the anisotropy-based ML correction with "true" DNS data.

- **Future Work**: We will focus on explainable machine learning models for turbulence closures utilizing SHAP (SHapley Additive exPlanations) & LIME (Local Interpretable Model-Agnostic Explanations) analysis.

Thank You for Your Time and Attention!

For questions or follow-up discussions:

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