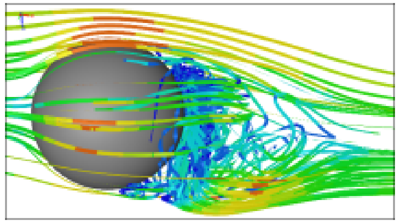
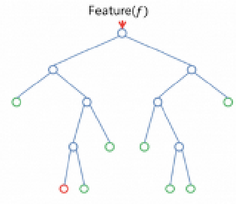
ASME-VVUQ 2024, May 15-17, Texas A&M, College Station

SAND2024-06089C

Sandia National Laboratories

Unraveling Sensitivity and Ensuring Reliability in Reynolds Stress Predictions for Data-Driven RANS





PRESENTED BY: Uma Balakrishnan

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

Sandia National Laboratories

ASC™ VERIFICATION VALIDATION

U.S. DEPARTMENT OF ENERGY NNSA

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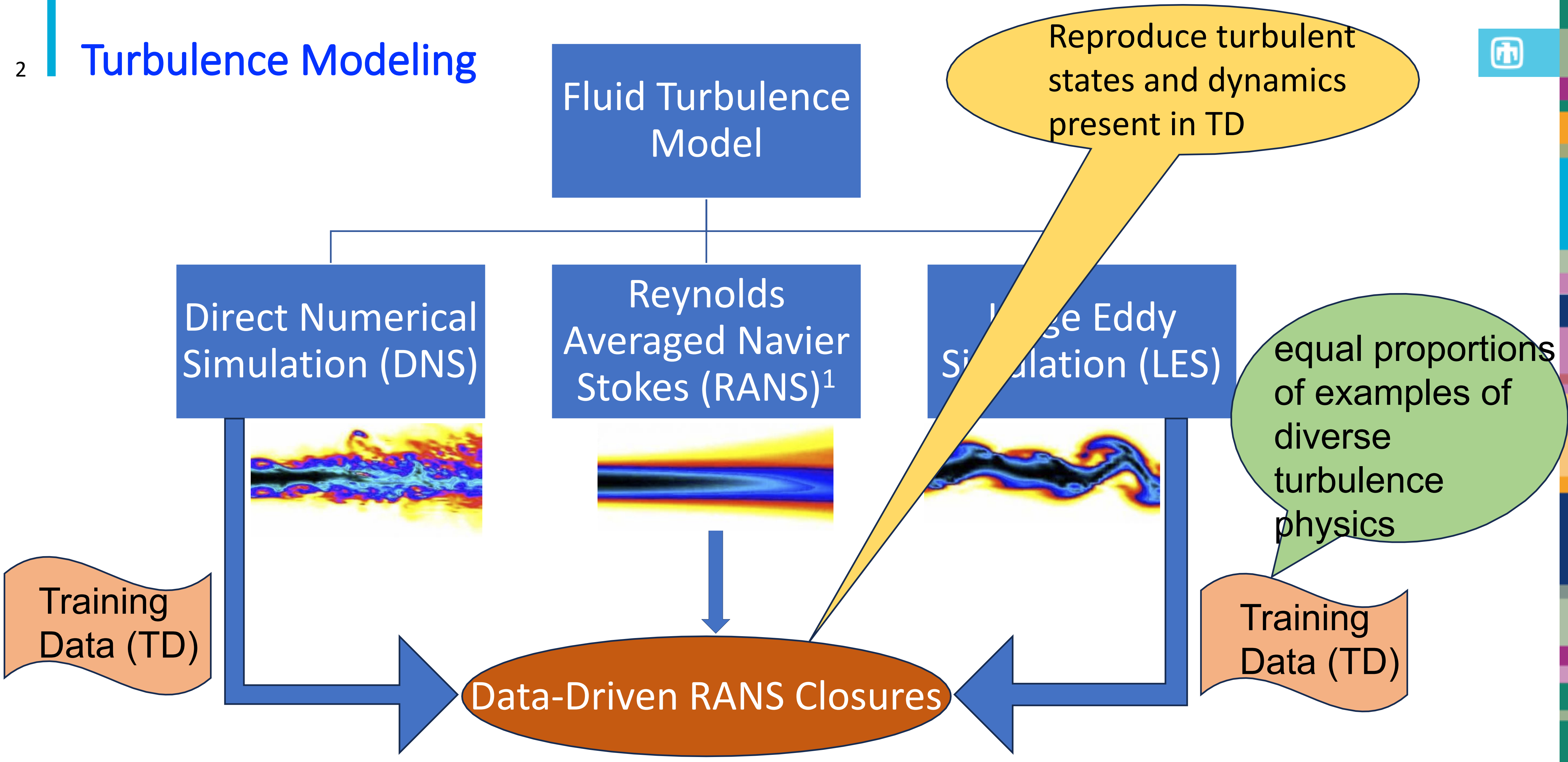
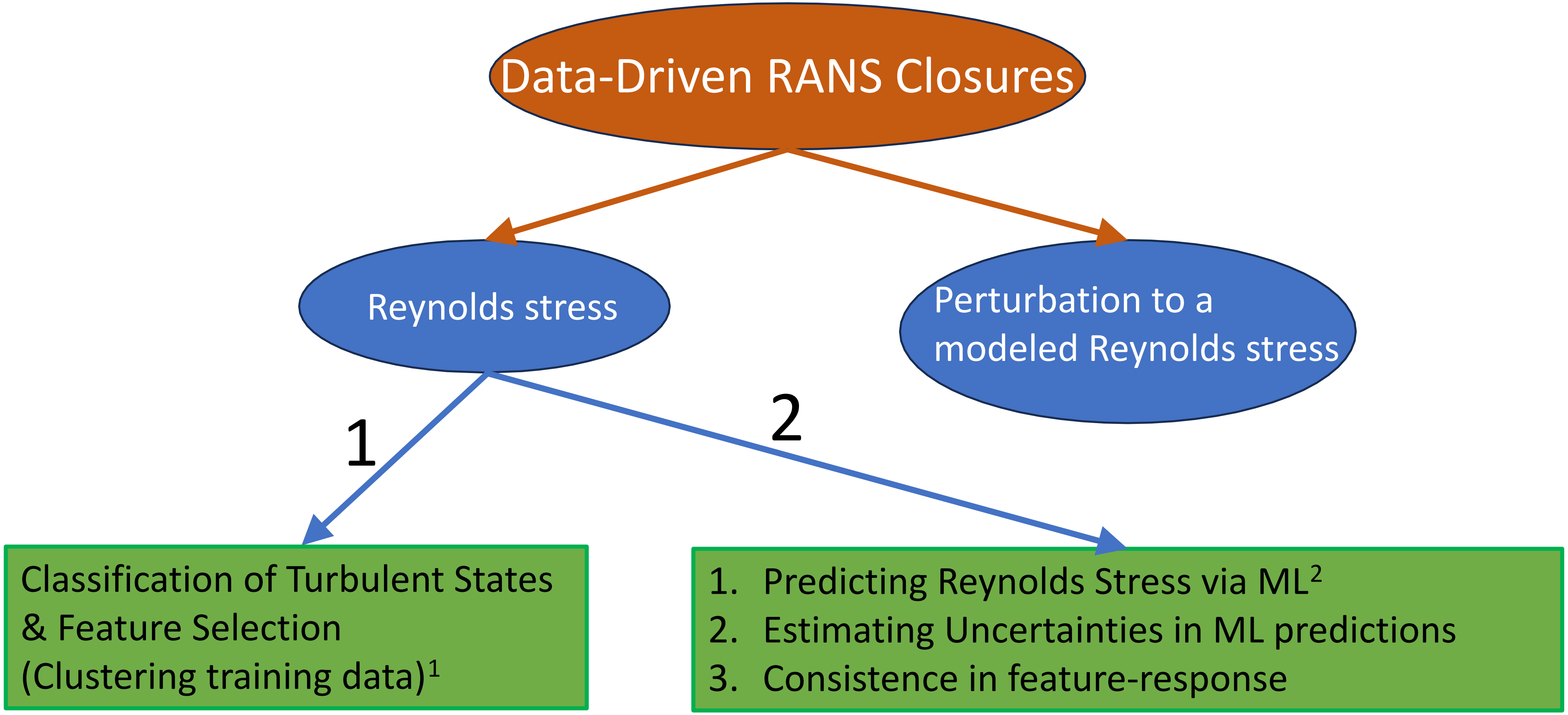
Turbulence Modeling



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.

Feature Subset and Optimal Clusters



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.

What is Credibility?

How do we demonstrate that **predictions** derived from computational simulations are **credible**?

Expert judgement, I have

Although aspects of these assertions may lend a certain level of credibility to analyses, these assertions cannot stand alone as the only credibility evidence to support a computational simulation prediction, particularly in a high-consequence environment

The computational simulation credibility process seeks to provide a documented, consistent, and repeatable process for assembling a comprehensive credibility evidence package to support computational simulation predictions

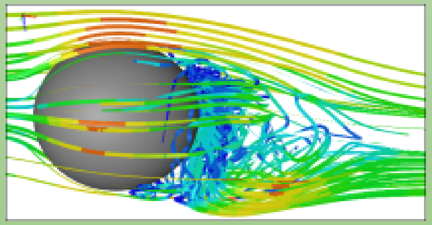
all of our calculations!

have never been
wrong before!

Motivating Credibility for Scientific Machine Learning (SciML)

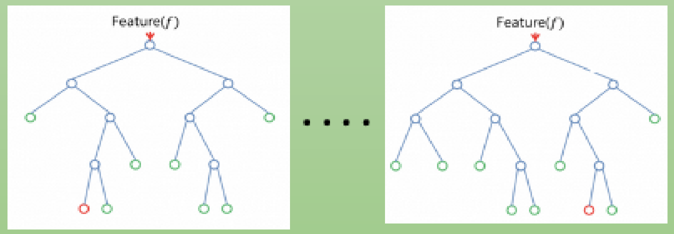
Machine learned models are used in lieu of, complementary to, or as surrogates for science and engineering computational simulation models.

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



Scientific Computing

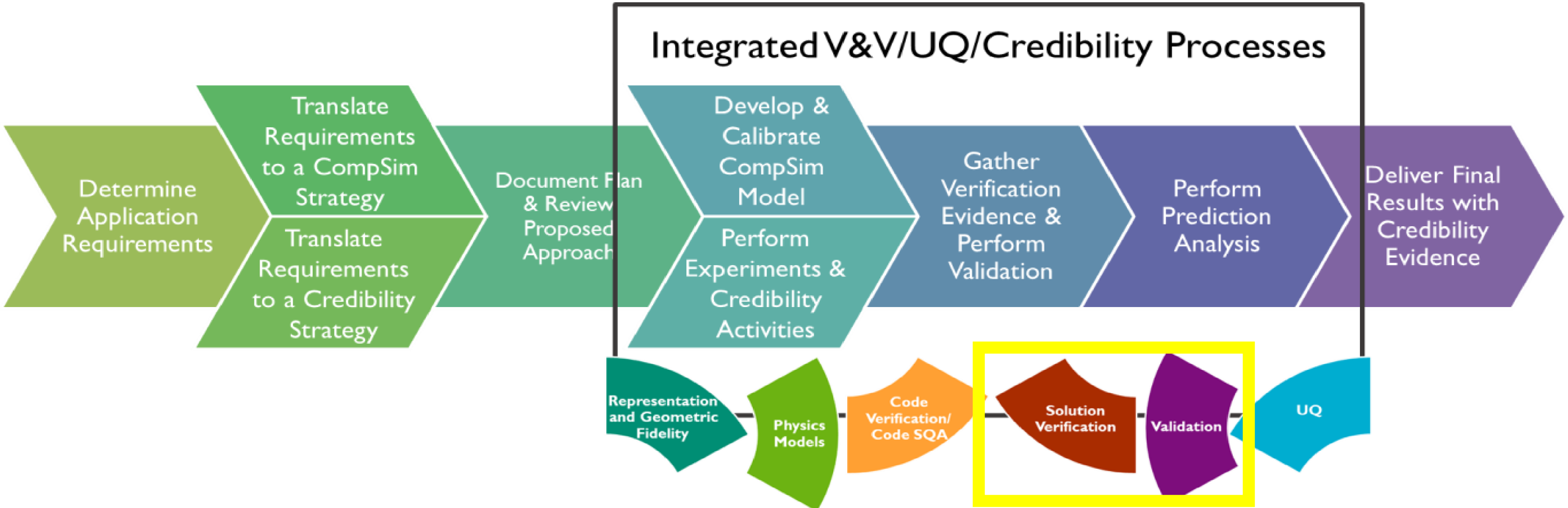
+



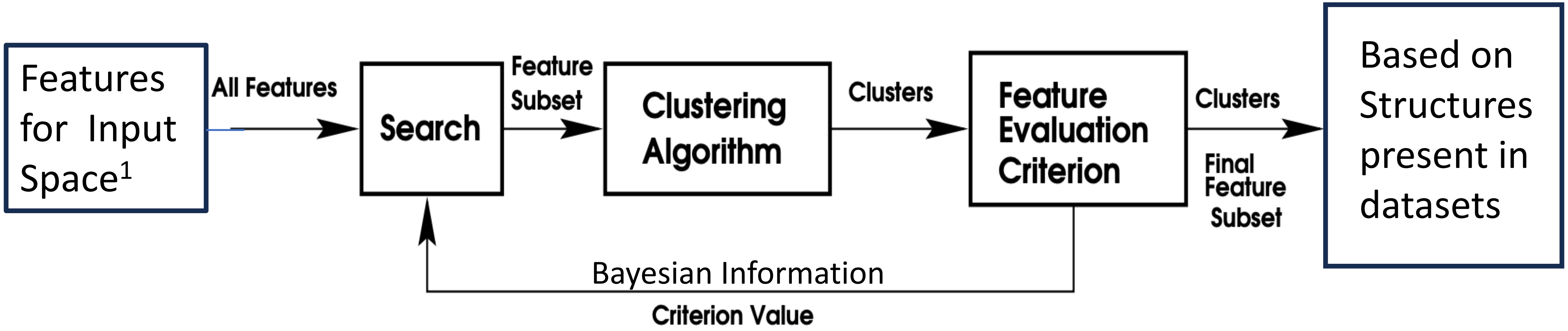
Machine Learning

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

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



Feature Subset and Optimal Clusters



Wrapper[3] approach to determine the best features and optimum number of clusters

3. Dy,J.G., and Brodley,C.E., "Feature Selection for Unsupervised Learning," *J. of Machine Learning Research*, Vol.5, 2004, pp. 845–889.

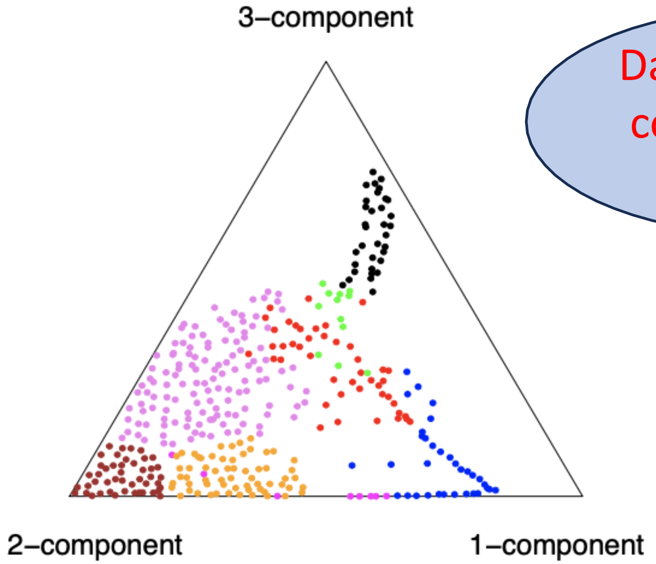
Why Clustering?

Solution Verification

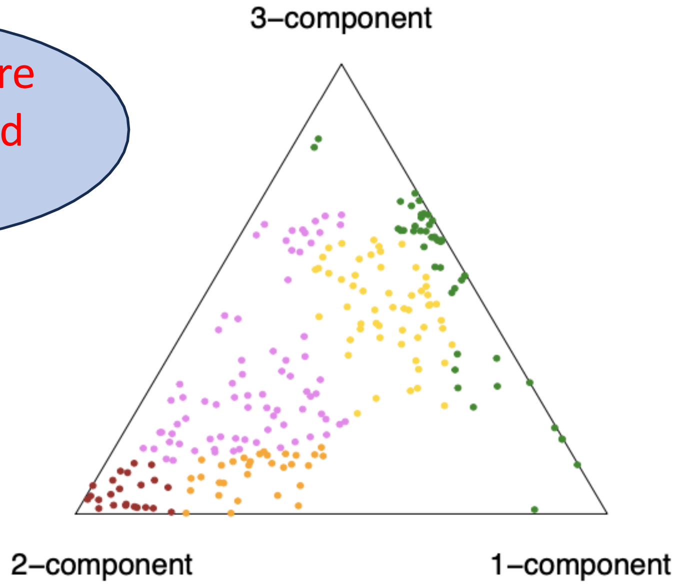
Automated partitioning of the training dataset into flow-field regions that reconcile with our human understanding of turbulent flow physics[1]

Candidate features that are Galilean and rotational invariant

Data points are colored based on clusters



Wavy Wall Flow



Square Cylinder in Cross-Flow

Is the training procedure for clustering algorithm credible?

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.

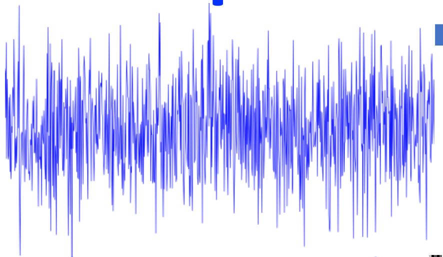
Sensitivity Analysis to the Performance of Clustering Algorithm

Solution Verification

QoI: Best Features &
Optimum number of Clusters

All Features

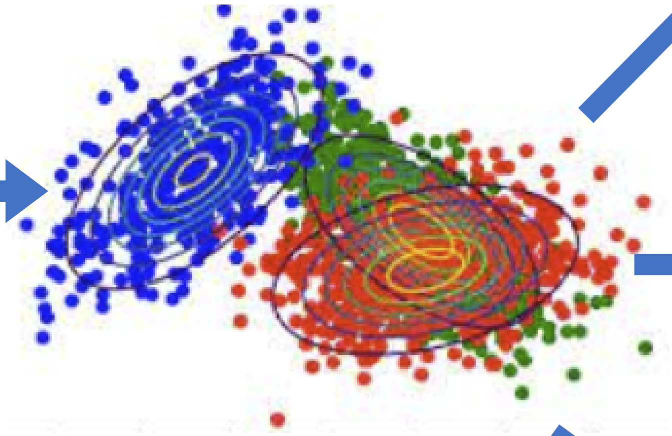
+

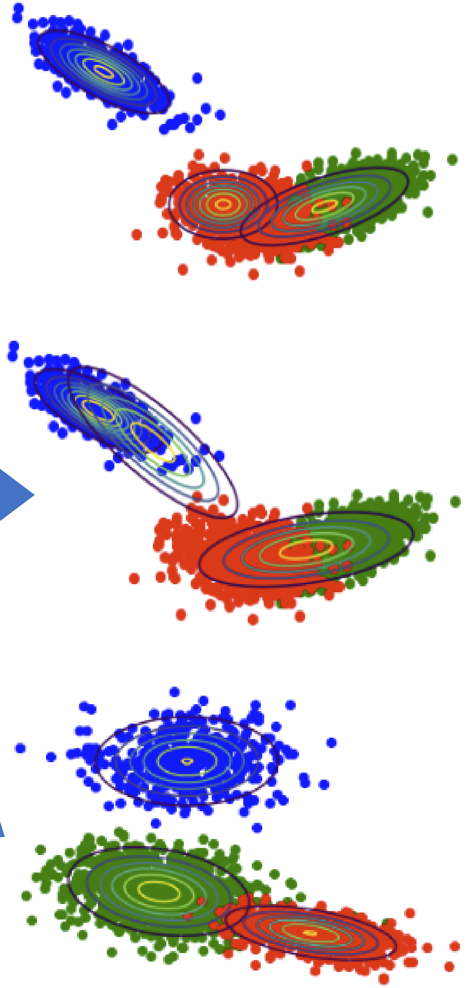


(White Noise) $f_i^n = f_i^n + noise_i^n$

Feature Search

Gaussian Mixture Model





$noise_i^n = \epsilon\, r[-1,1]\, std(f_i^n),\ noise_i^n < std(f_i^n)$

(Globally Scaled Noise)

$noise_i^n = \epsilon\, r[-1,1]\, f_i^n,\ noise_i^n < f_i^n$

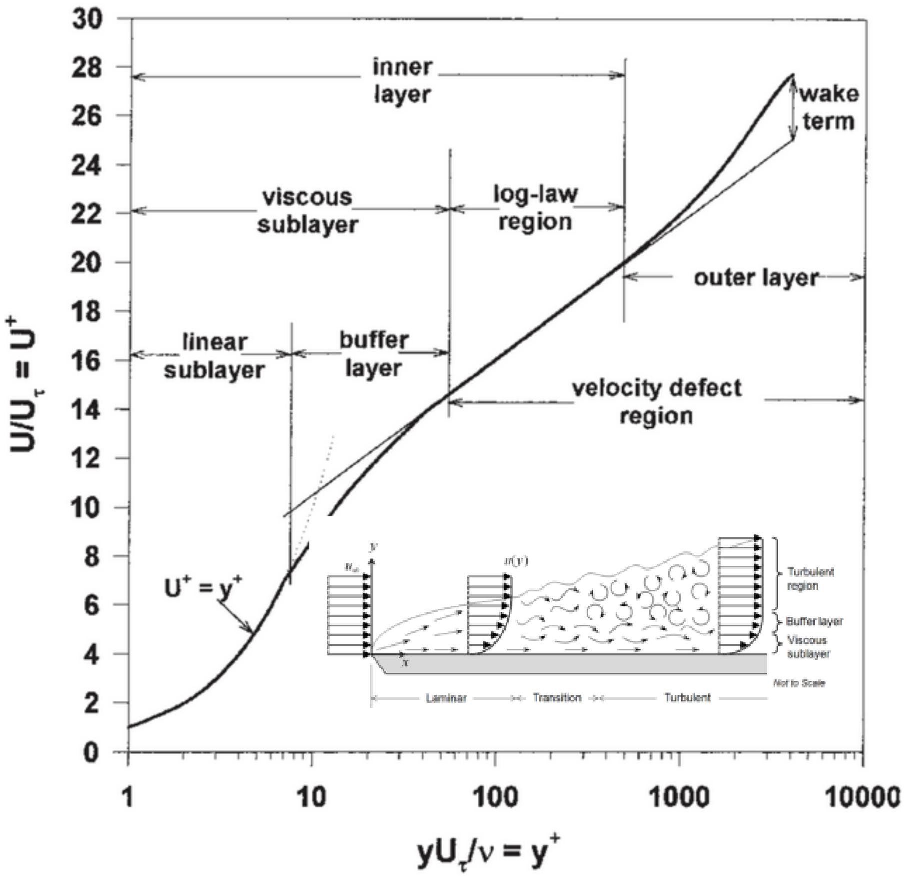
(Locally Scaled Noise)

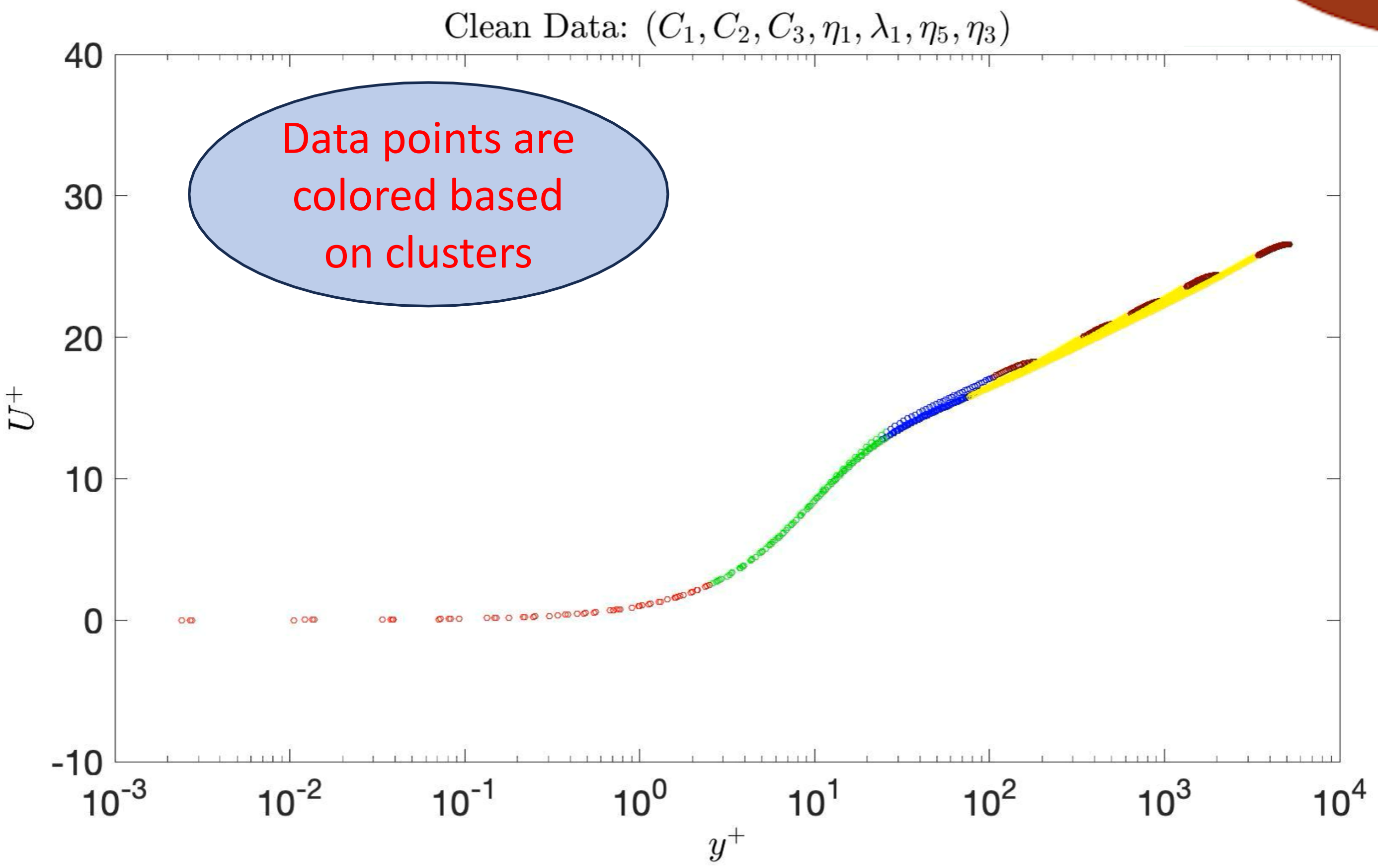
$$noise_i^n = \epsilon\, r[-1,1] \frac{\sum_{i \in N\ neighbor} f_i^n}{N},\ noise_i^n < f_i^n$$

(Locally Scaled Noise by Neighborhood)

Plane Channel Flow

Solution Verification





- ➢ The clustering algorithm is sufficiently robust in identifying best features and number of optimal clusters for Plane Channel Flow.

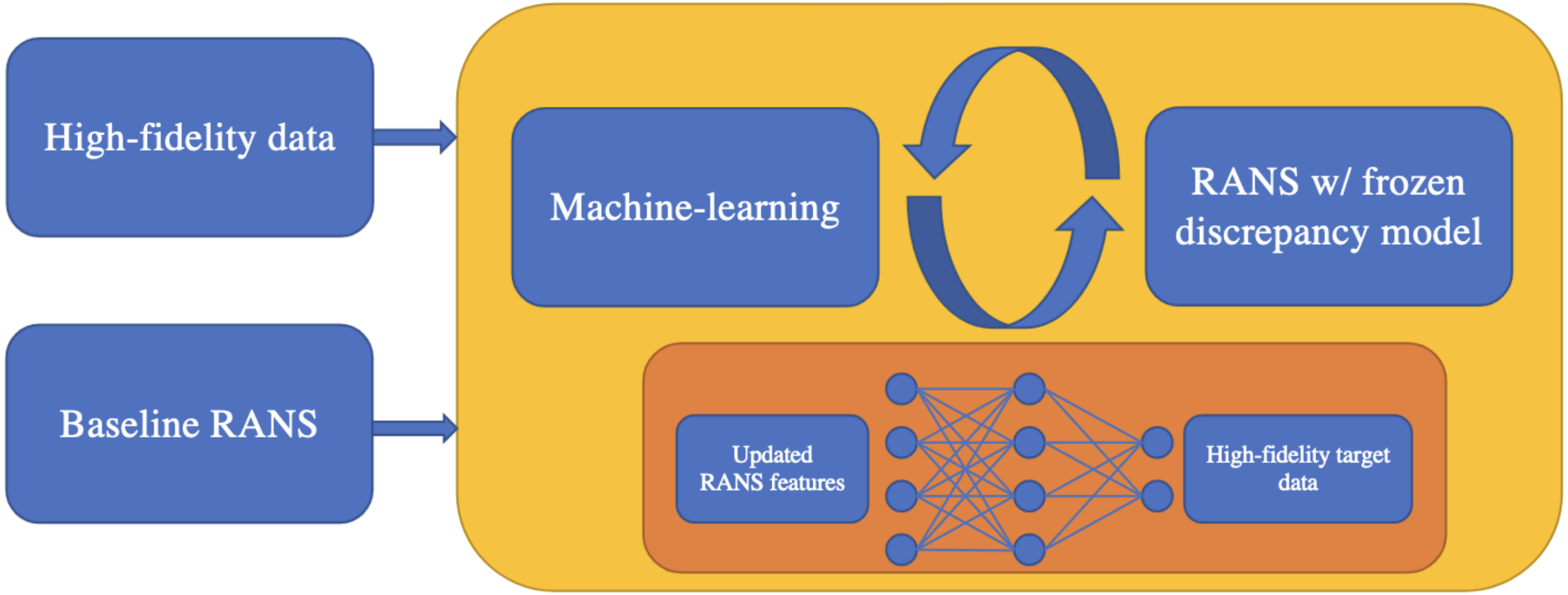
Data-Driven Turbulence Modeling

$$a_{ij} \approx a_{ij}^{\mathrm{RANS}} + m_{ij}^{\mathrm{ML}}$$ Anisotropy-based discrepancy term

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

$$a_{ij}^{\mathrm{RANS}} = \frac{\tau_{ij}^{\mathrm{RANS}}}{2\bar{\rho}\tilde{k}} - \frac{1}{3}\delta_{ij}$$ Anisotropy tensor predicted by a standard RANS

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



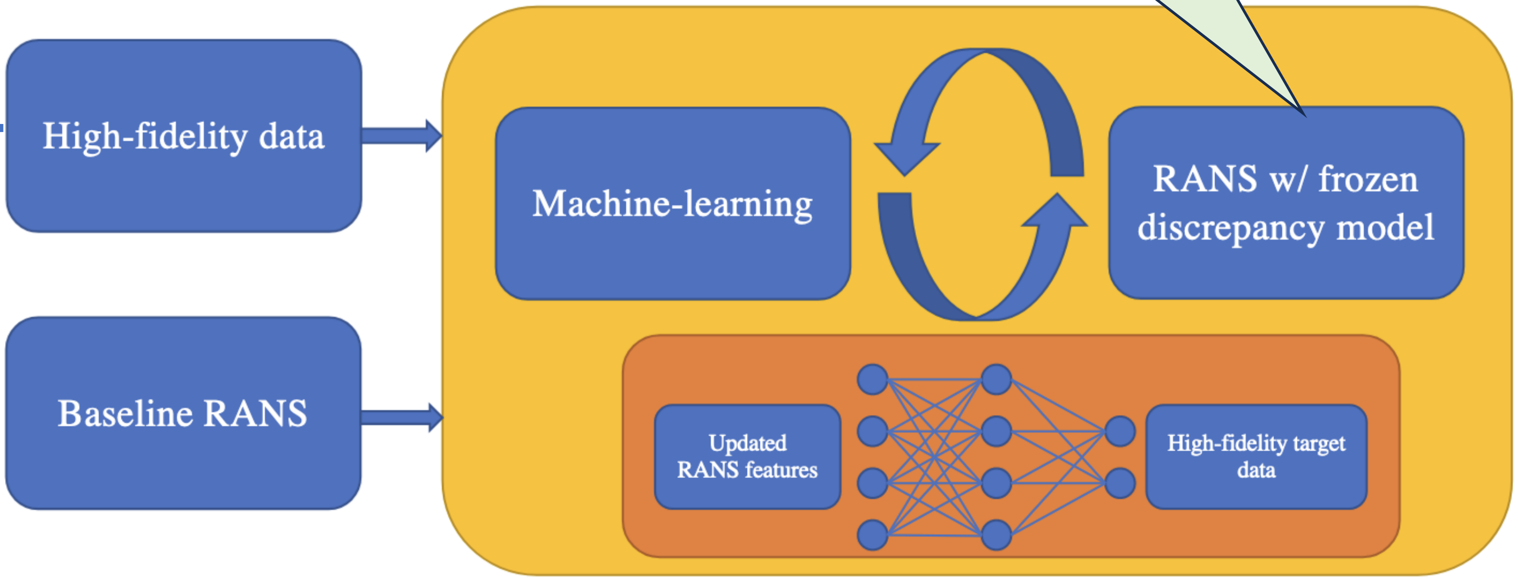
2. E. Parish, D.S. Ching, N.E. Miller, S. J. Beresh and M. F. Barone. "Turbulence modeling for compressible flows using discrepancy tensor-basis neural networks and extrapolation detection," AIAA 2023-2126. *AIAA SCITECH 2023 Forum*. January 2023.

Data-Driven Turbulence Modeling

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

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, $T_w/T_r = 0.18$



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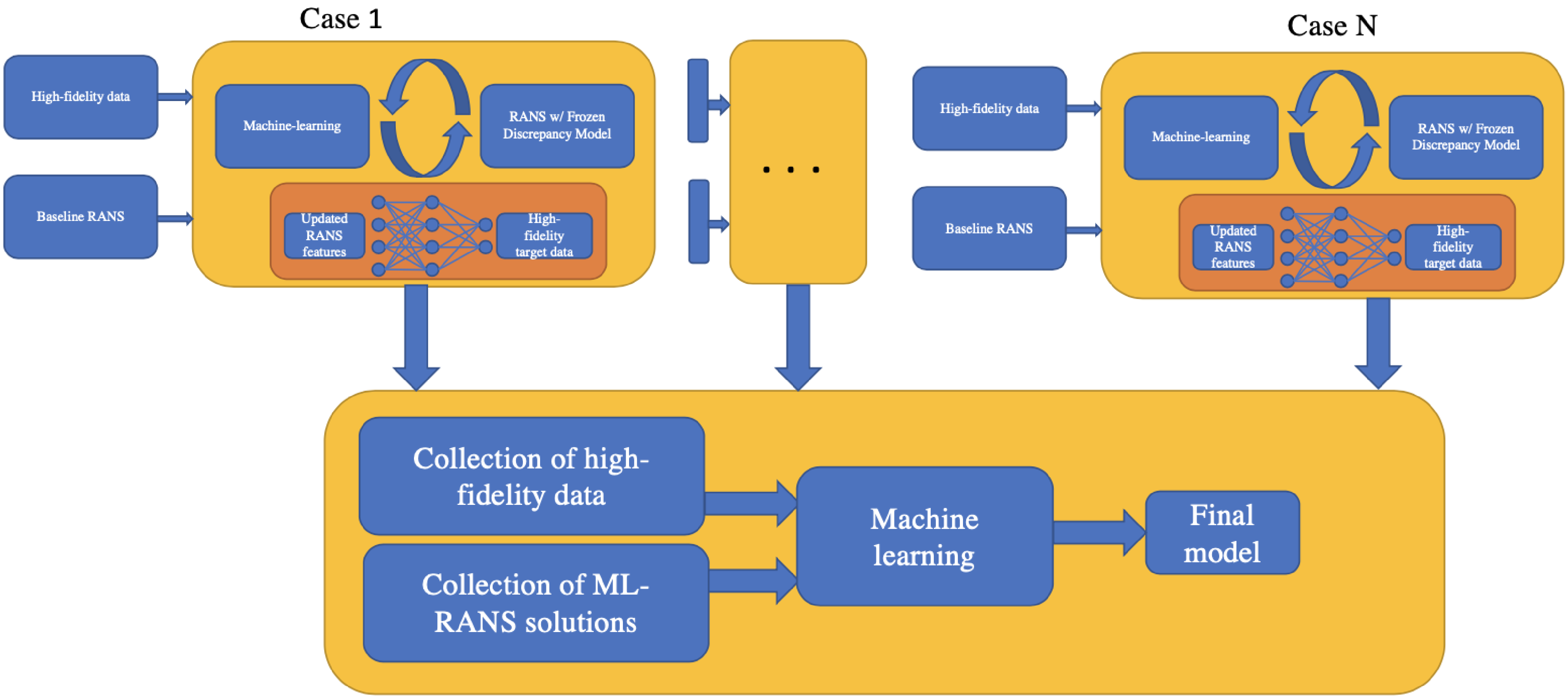
Global Training Process



Data-Driven Turbulence Modeling

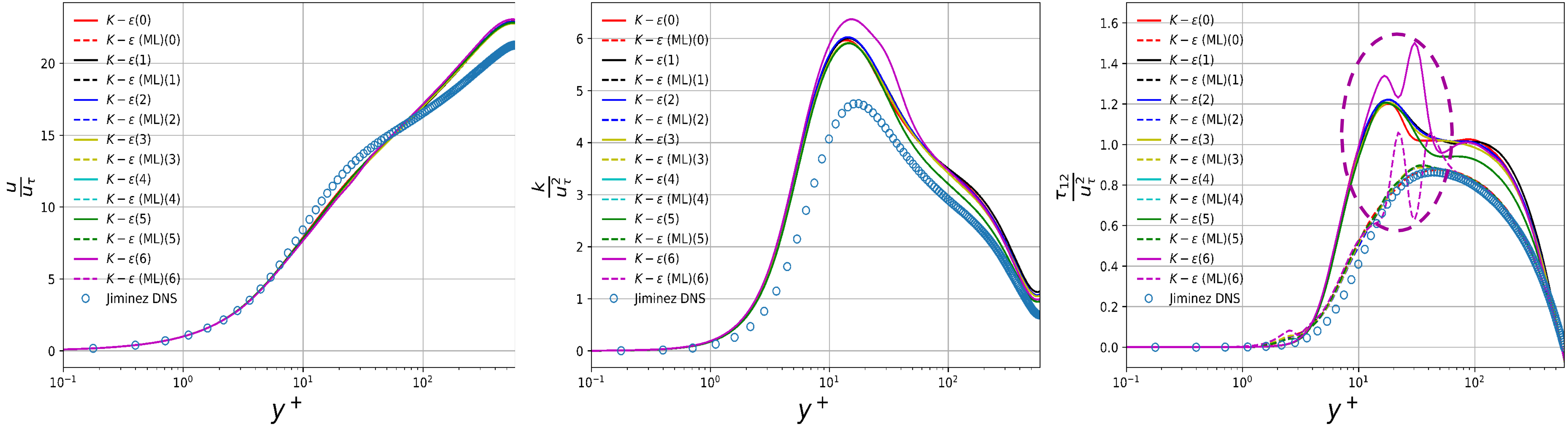
- Global iterative training procedure improves feature consistency.
- Complete consistency in response has not been achieved.
- The goal is to minimize overall inconsistency.
- ML models involve many hyperparameters.
- Considering various combinations of training datasets and testing hyperparameters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

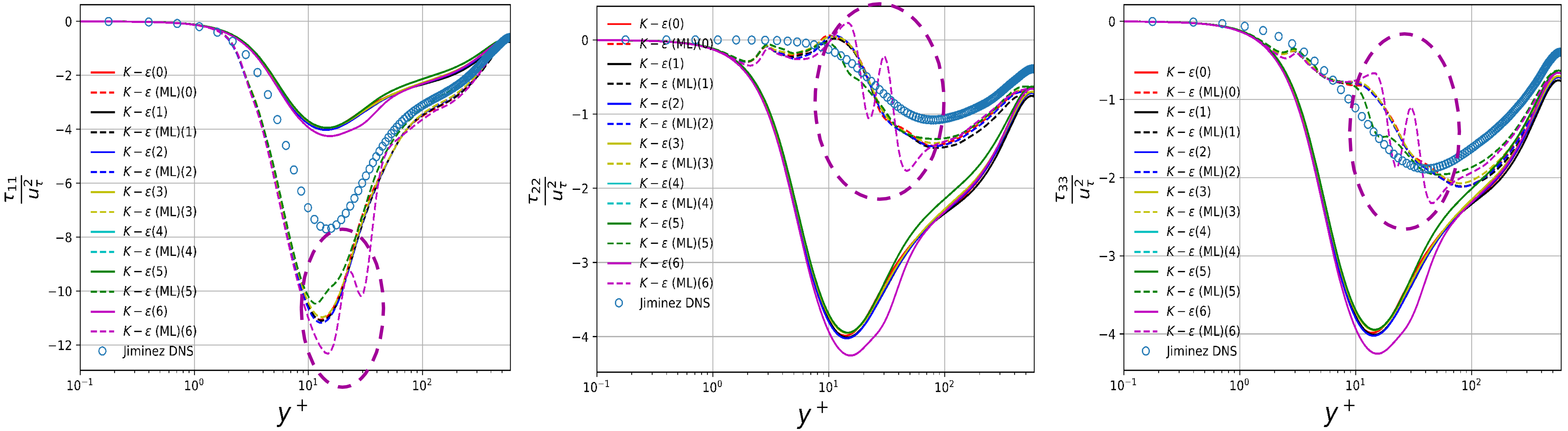
Validation of Training Datasets / Procedure & Testing



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.

Validation of Training Datasets / Procedure & Testing

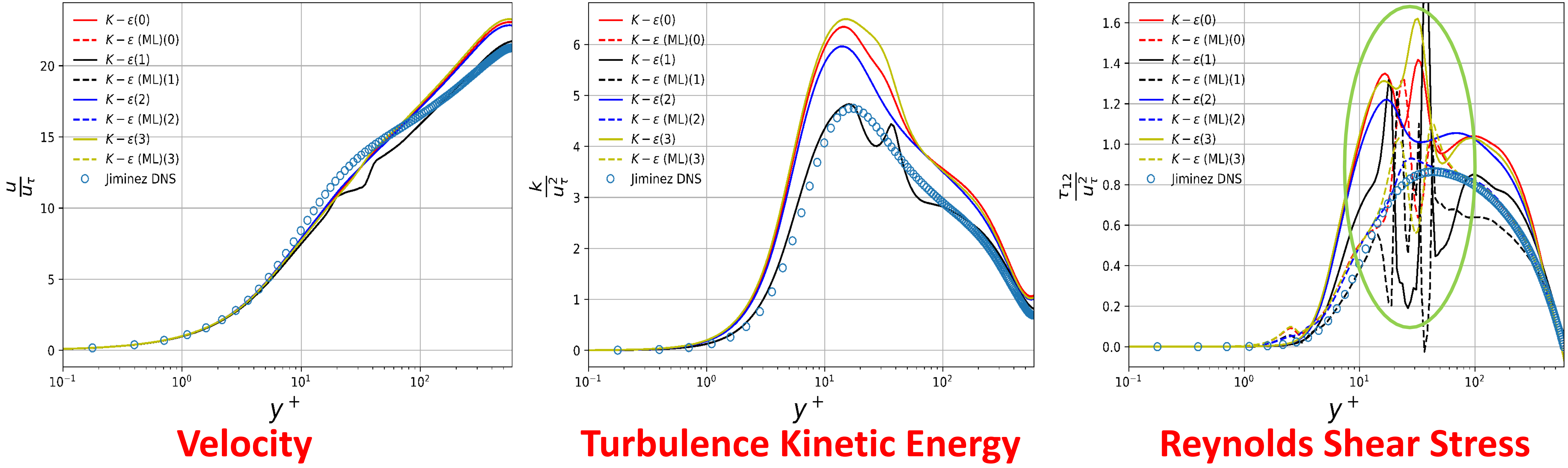


Normal Stress in x, y & z direction

- 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.

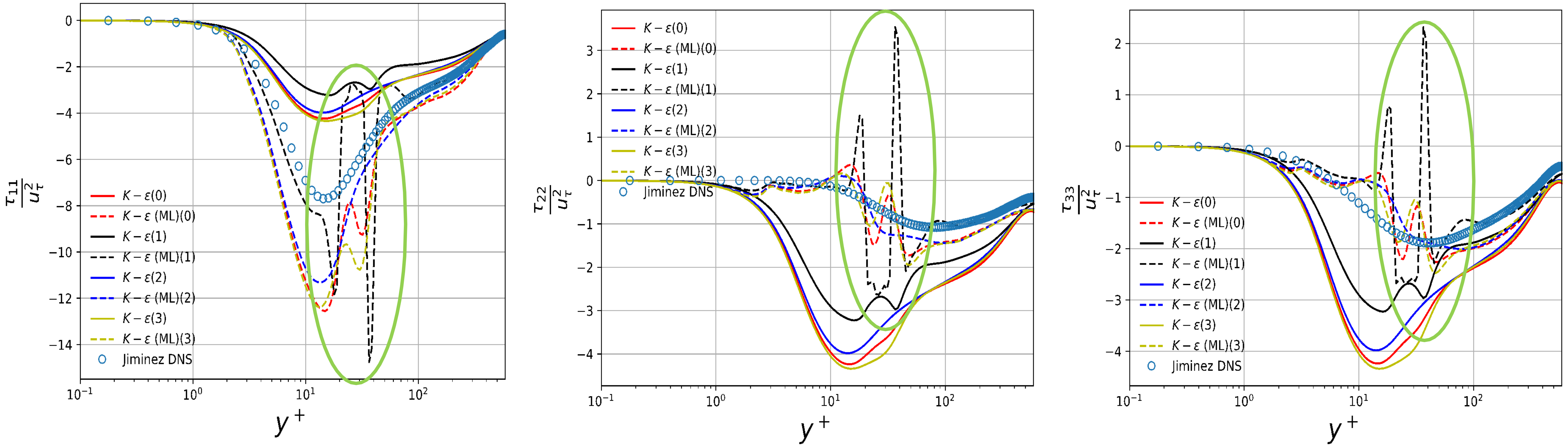
- Dataset combination (6) exhibits clear oscillations.

Combination of Training Dataset (6)



(0) No change in hyperparameters, (1) Number of epochs increased (overfitting), (2) Reduced depth of NN (better convergence), (3) Reduced width of NN.

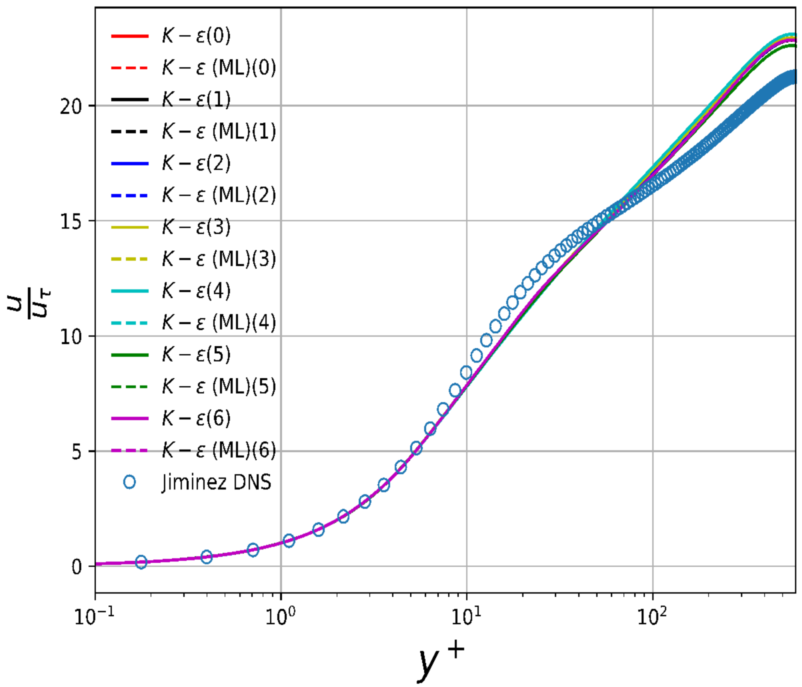
Combination of Training Dataset (6)



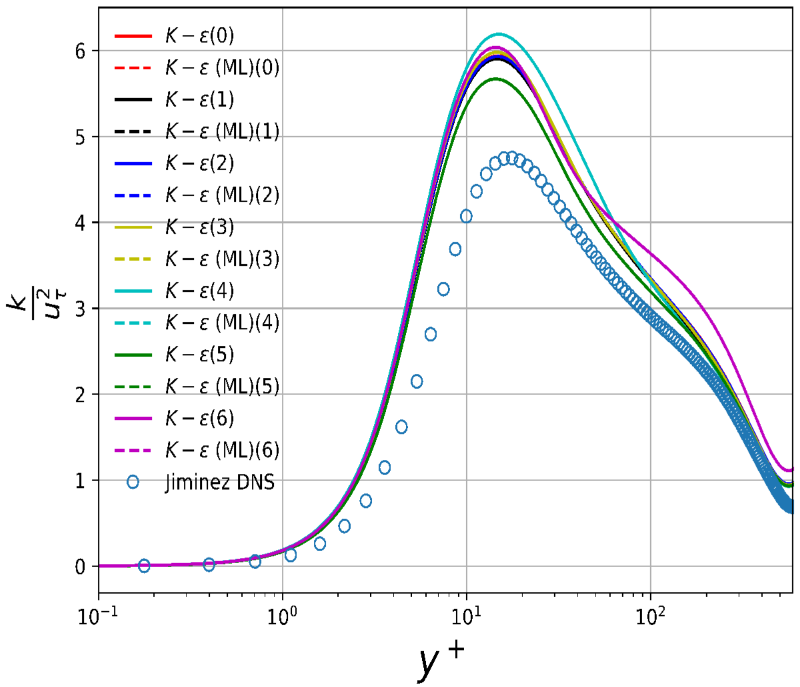
Normal Stress in x, y & z direction

(0) No change in hyperparameters, (1) Number of epochs increased (overfitting), (2) Reduced depth of NN (better convergence), (3) Reduced width of NN.

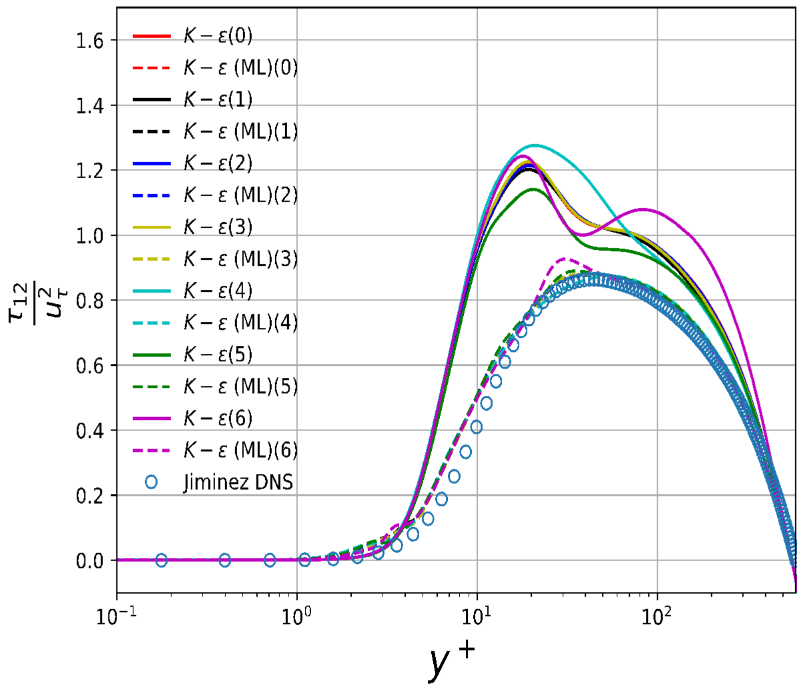
Reduced Depth & Width of Neural Network



Velocity



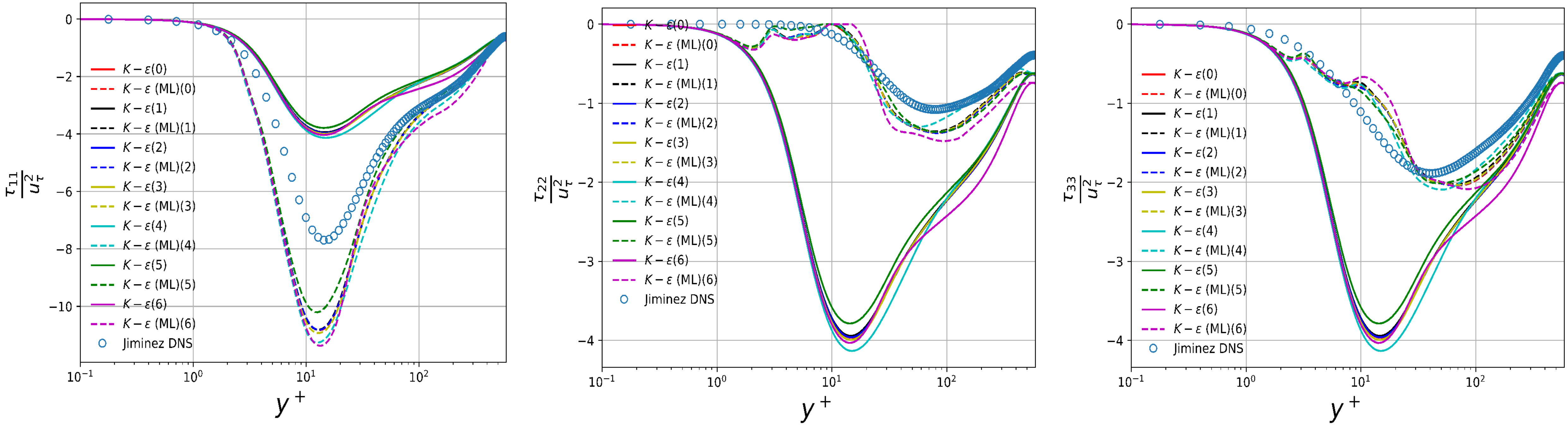
Turbulence Kinetic Energy



Reynolds Shear Stress

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

Reduced Depth & Width of Neural Network



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.

Conclusions and Future Work

- **Performance Consistency**: The training procedure demonstrates strong performance across various combinations of training datasets, aligning well with the trends of true datasets when tested on in-distribution datasets.

- **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 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 Testing Strategy**: Moving forward, we plan to conduct rigorous testing on a variety of in-distribution and out-of-distribution datasets using different combinations of training datasets.

Thank You for Your Time and Attention!

For questions or follow-up discussions:

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