Physics-Informed Machine Learning for Data-Driven Turbulence Modeling

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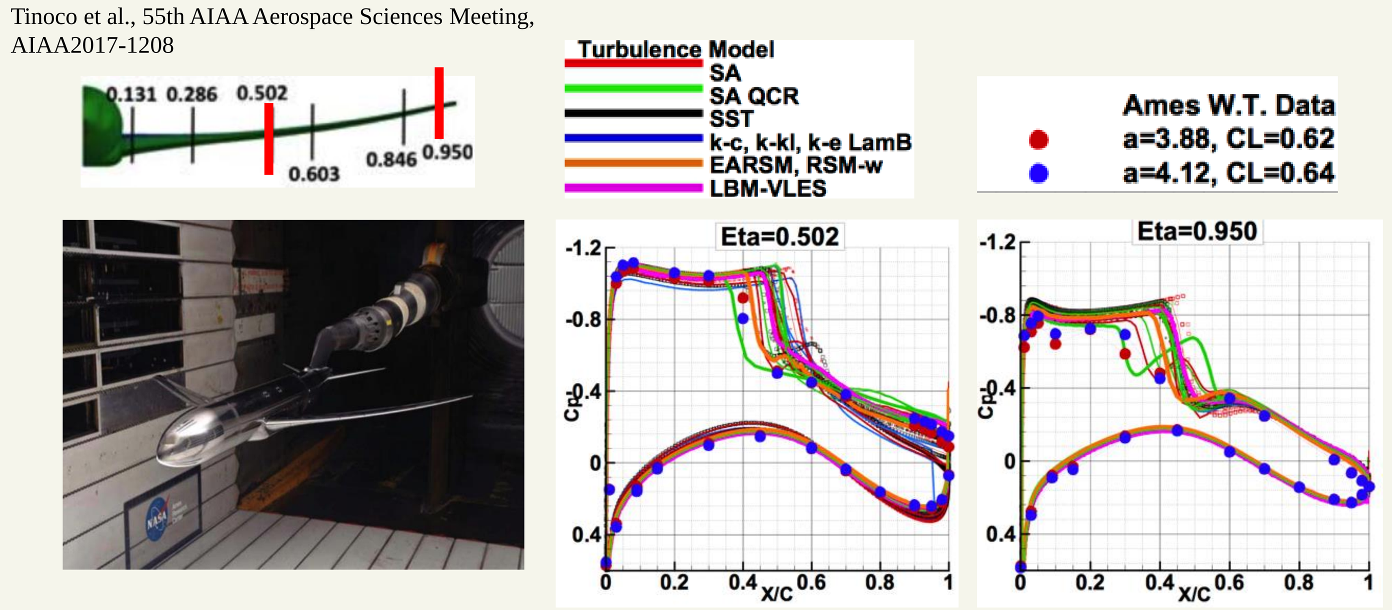
Motivation

Reynolds Averaged Navier-Stokes Equations:

$$\frac{\partial U_i}{\partial t} + \frac{\partial (U_i U_j)}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} = \boxed{\nabla \cdot \tau} \qquad \tau = -\overline{u_i' u_j'}$$

Hub of RANS models

Tinoco et al., 55th AIAA Aerospace Sciences Meeting, AIAA2017-1208



Our Motivation:

- ❑ RANS modeled Reynolds stresses are known to be unreliable for many flows.
- ❑ LES/DNS simulations are still infeasible for many industrial flows.
- ❑ Is it possible to employ existing LES/DNS database to enhance the RANS simulations?

Objective and Approach

The objective of this work is to demonstrate that the RANS simulated Reynolds stress of a new flow can be improved via our PIML framework with existing LES/DNS database. Three essential parts of our PIML framework is: (1) **invariant** representation of Reynolds stresses discrepancies as outputs; (2) identification of **invariant** mean flow features as inputs and (3) construction of a machine learning model to discover the functional mapping from inputs to outputs of training data.

(1) Representation of Reynolds Stresses as Responses

$$\frac{\partial U_i}{\partial t} + \frac{\partial (U_i U_j)}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} = \nabla \cdot (\tau_{RANS} + \Delta\tau)$$

$$\tau = 2k\left(\frac{1}{3}\mathbf{I} + \mathbf{A}\right) = 2k\left(\frac{1}{3}\mathbf{I} + \mathbf{V}\Lambda\mathbf{V}^T\right)$$

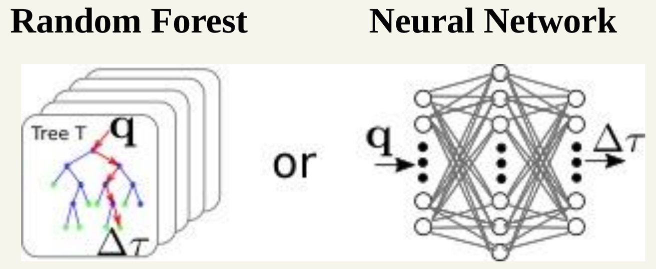
$$\boxed{\Delta\tau \Rightarrow (\Delta \log_2 k, \Delta\xi, \Delta\eta, \Delta\mathbf{V}_1, \Delta\mathbf{V}_2, \Delta\mathbf{V}_3)}$$

(2) Identification of Mean Flow Features

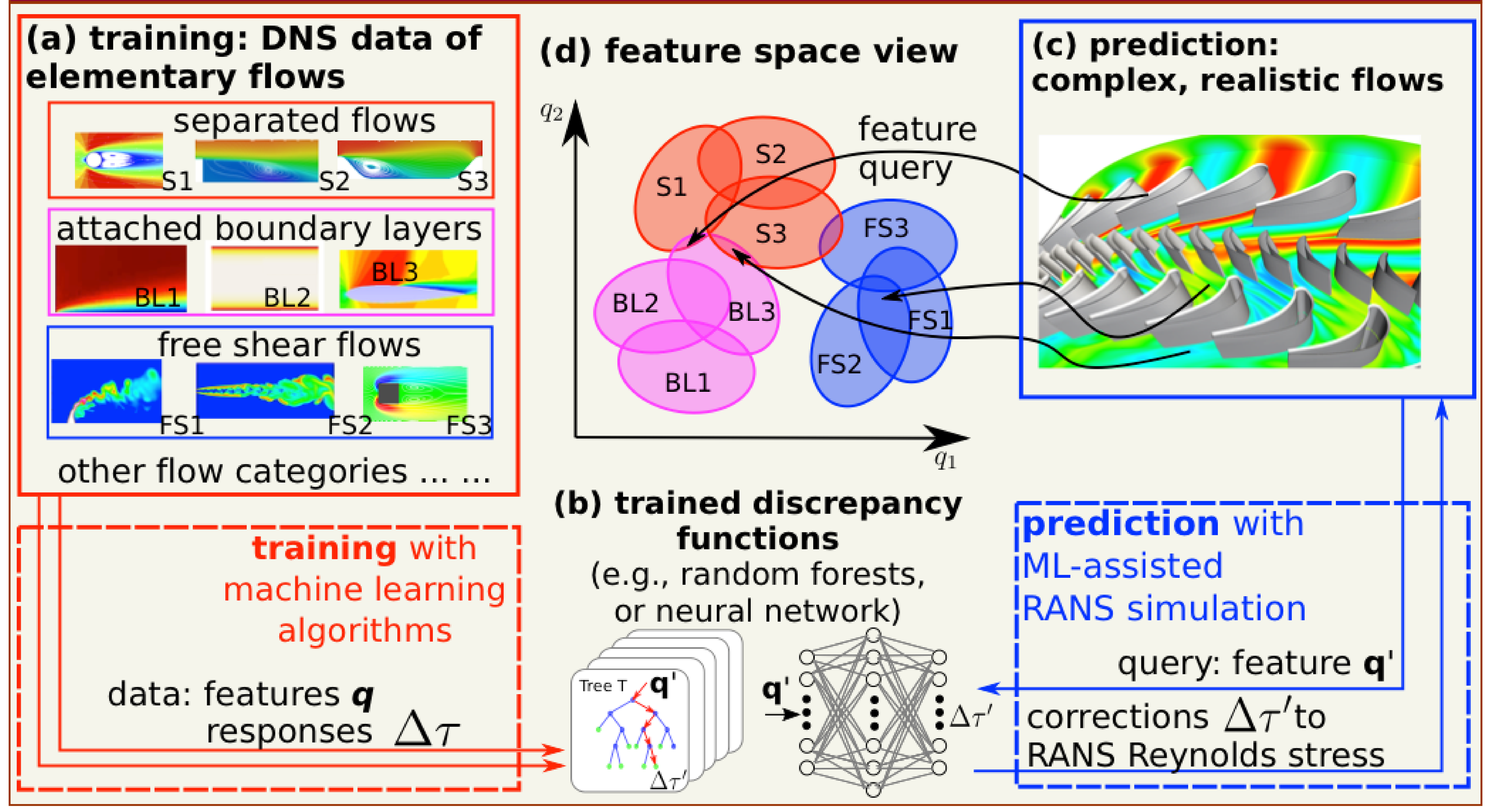
Integrity Basis of $\{\mathbf{S}, \boldsymbol{\Omega}, \nabla p, \nabla k\} \Rightarrow \boxed{\mathbf{q}_i \ (i = 1, 2, ..., 47)}$

(3) Construction of Regression Functions

Random Forest **Neural Network**



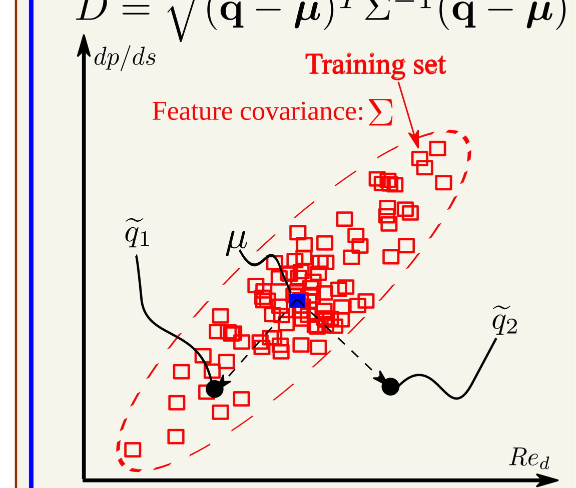
Physics-Informed Machine Learning Framework



Statistical Metrics

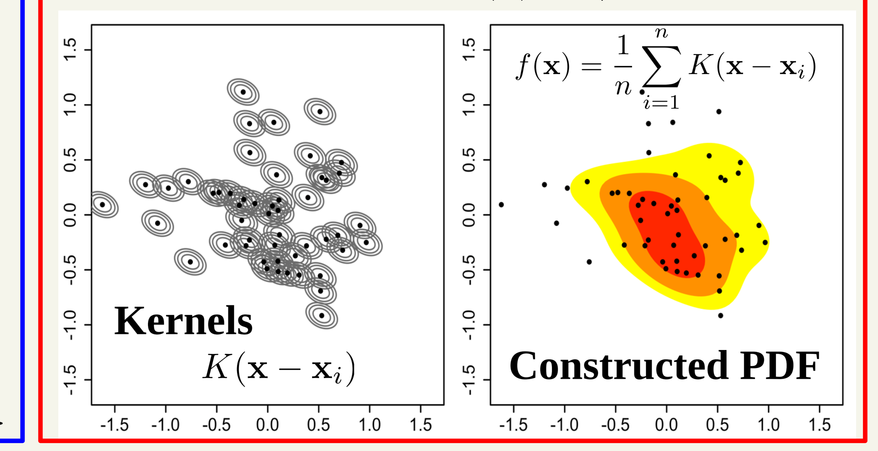
(1) Mahalanobis Distance:

$$D = \sqrt{(\tilde{\mathbf{q}} - \boldsymbol{\mu})^T \Sigma^{-1} (\tilde{\mathbf{q}} - \boldsymbol{\mu})}$$



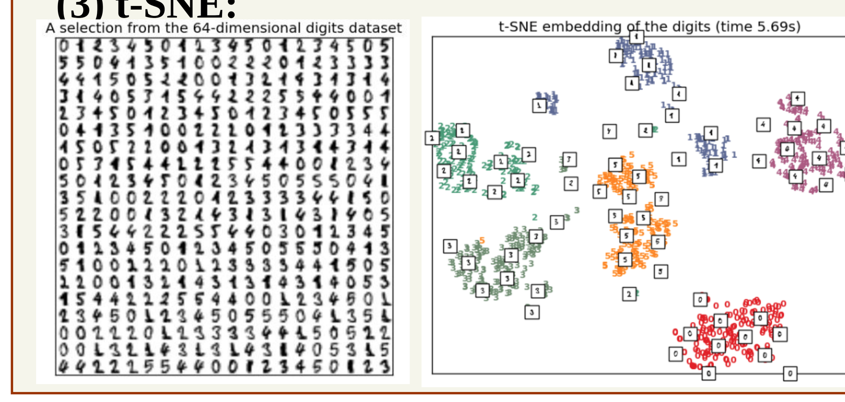
(2) KDE Distance:

$$D_{KDE} = 1 - \frac{f(\mathbf{x})}{f(\mathbf{x}) + 1/A}$$



$$f(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} K(\mathbf{x} - \mathbf{x}_i)$$

(3) t-SNE:



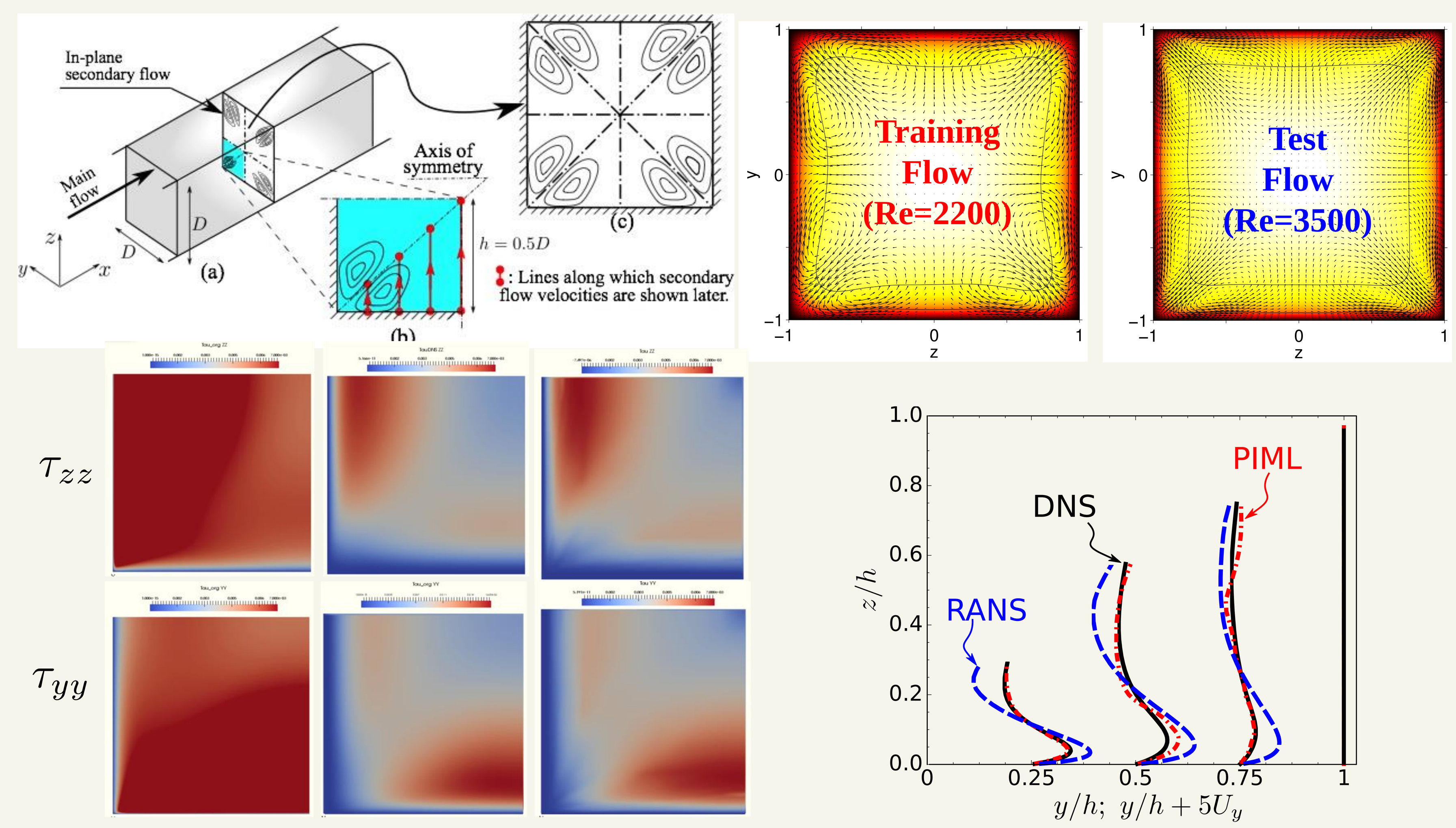
$$p_{j|i} = \frac{\exp\left(\|x_i - x_j\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-\|x_i - x_k\|^2 / 2\sigma_i^2\right)}$$

$$q_{j|i} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq i}(1 + \|y_i - y_k\|^2)^{-1}}$$

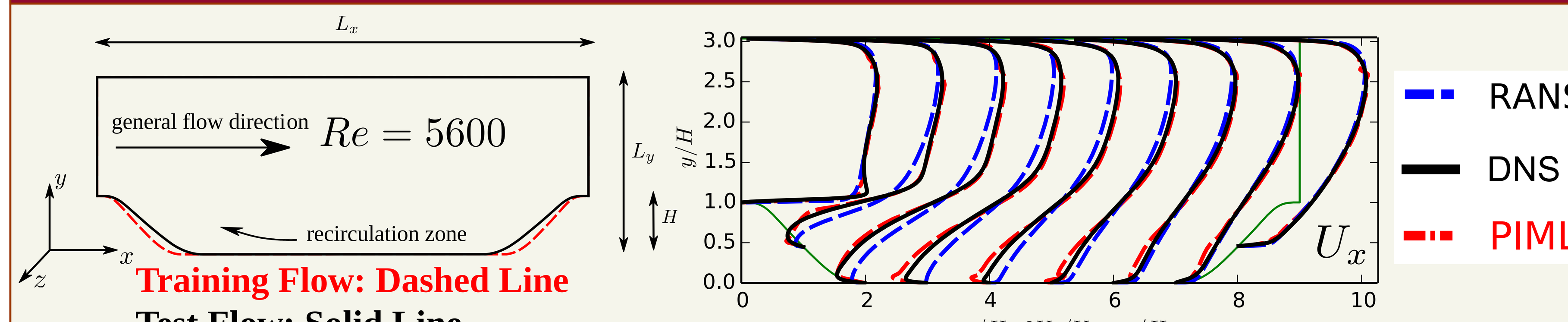
Minimize:

$$C = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

Application I. Flow in A Square Duct

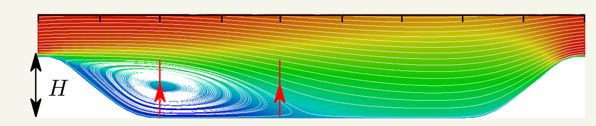


Application II. Flow over Periodic Hills

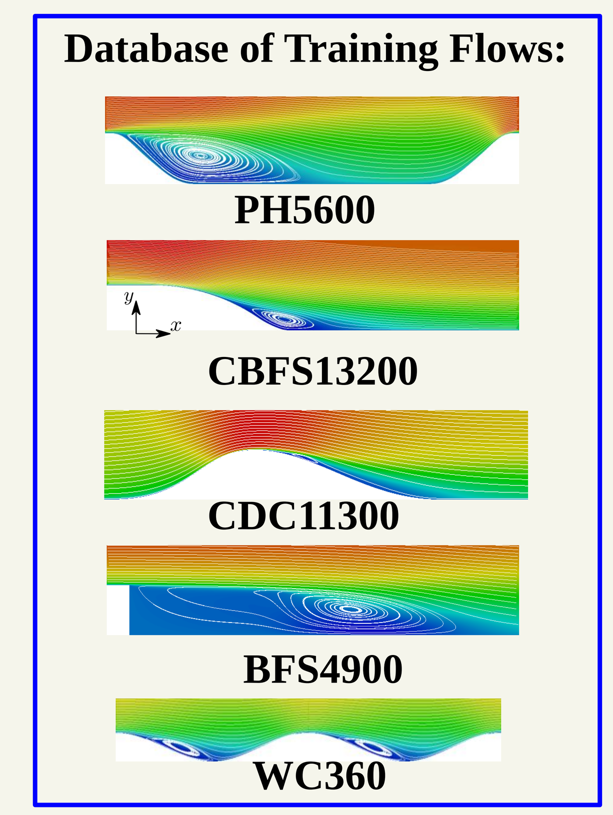


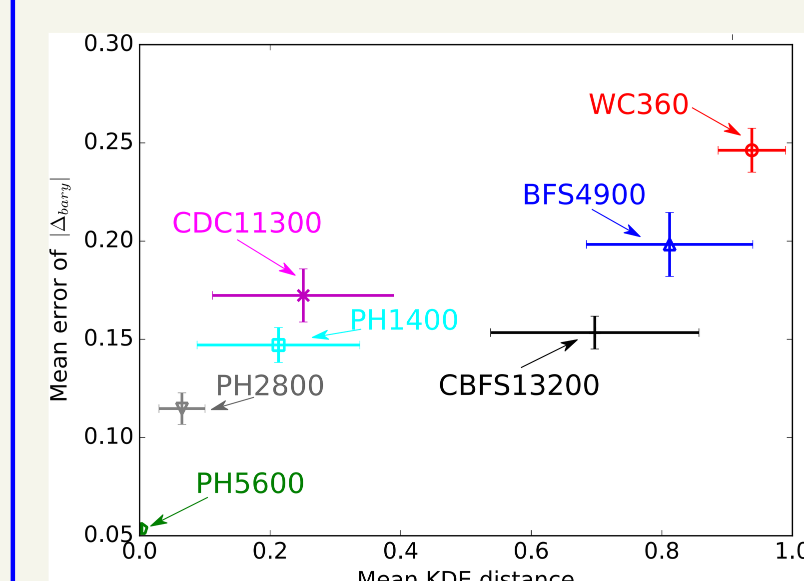
A Priori Assessment

Test Flow: Periodic hills, Re=10595



- ❑ The prediction performance depends on the choice of the training flows.
- ❑ In real applications, the true quantities of the test flow are usually unknown.
- ❑ We use statistical metrics to assess the prediction confidence *a priori*.





Conclusions

In this work, we proposed a physics-informed machine learning (PIML) approach to predict RANS modeled Reynolds stresses discrepancies by utilizing DNS database. The potential impacts include:

- ❑ Utilizing current high-fidelity simulations database to improve the accuracy of RANS simulations
- ❑ Assisting turbulence modelers to derive better RANS models
- ❑ Inspiring other data-driven modeling approaches in computational mechanics

Bibliography

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Further Information

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