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Application of Physics Informed Machine Learning model for correcting RANS modeled Reynolds Stress Anisotropy

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1. Summary:

The physics informed machine learning (PIML) approach in our research is aimed to enhance the accuracy of an-isotropic component(A) of Reynolds Stress tensor (R) modelled by Reynolds Averaged Navier Stokes (RANS) based turbulence models. The framework, which is referenced from Wang et.al[1], is completely developed and applied for 2D backward facing step (BFS) and the eigen space projected corrections of A are illustrated using barycentric representation[2], for wall normal 1D line predictions, to better correlate the aspects of turbulent flow physics. In addition, framework is extended for correcting RANS modeled anisotropic tensor in full scale 2D simulations and the preliminary results are presented. Decision trees based random forest (RF) and neural network (NN) models are used. Although the accuracy of both approaches is similar with respect to flow physics in barycentric representation, the execution time (training and prediction) for NN based model is significantly higher for the considered Computational Fluid Dynamics (CFD) simulations data set. The framework is being extended further based on the concluded observations.

2. Introduction:

RANS turbulence modeling based CFD, even though it is less accurate, is the work horse methodology to analyze fluid flow physics for industry relevant practical cases. However, their inaccuracy majorly arises from the specific closure modeling approach used to compute non-linear Reynolds stress term resulted from RANS equations. First moment closure Models like Spalart-Allmaras, k-ε, k-ω etc. assumes linear relationship between R and mean strain rate, resulting from Boussinesq hypothesis. Although, second moment closure models like Reynolds stress models solve for individual components of R, they result in the necessity to model for even more number of unknowns requiring higher computational resources. All such forms of modeling can result in ill-prediction of R, which includes second order fluctuating velocity terms $u'_i u'_j$ with RANS representation of instantaneous velocity as $U = \overline{U} + u'$. Specifically, RANS equations based models have significant limitations in modeling anisotropic components of R which results in inaccurate top level CFD flow fields like velocity, pressure etc. Hence, our research is focused on correcting this anisotropy component of R, using data driven machine learning models incorporated with input features and responses containing detailed physics information.

3. Computational Models:

The 2D backward facing step [5] case is computed using RANS and DNS at Reynolds number (Re) of 32k which is used to train both RF and NN based ML models. The test case consists of only RANS data at Re 36k and the ML predictions are validated with un-used DNS data computed at same Reynolds number.

a. Computational Fluid Dynamics (CFD)

CFD simulations are performed using an open source solver framework OpenFOAM [3] within which steady-state RANS simulations are computed by k-Epsilon turbulence model using SIMPLE pressure - velocity coupling algorithm and transient DNS simulations using PISO algorithm. Second order spatial and temporal discretization schemes are used for structured 2D grid, generated with another open-source tool gmsh[4].

b. Machine Learning (ML)

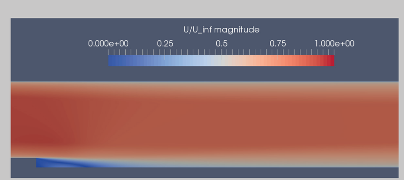
The ML model is provided with the training data along only localized wall normal lines shown in figure 1(a) and the predictions are done in the same locations. The inputs are derived from pressure, velocity, turbulent kinetic energy, energy dissipation rate, strain and rotation rate. For example, inputs include pressure gradient along streamline, ratio of convection to production of turbulent kinetic energy etc. totaling 10 parameters [1]. The responses (ξ) and (η) are derived from Eigen values of an-isotropic tensor (A) which are represented in the barycentric triangle [1]. The Eigen decomposition includes.

$$A=(R/2k)-\ I/3 \ \Rightarrow V\lambda\, V^T$$

Where k = turbulent kinetic energy (trace(R)), I = identity matrix, $V=[v_1\ v_2\ v_3]$ are Eigen vectors and $\lambda=\mathrm{diag}[\lambda_1\ \lambda_2\ \lambda_3]$ are Eigen values. With $\xi= \sqrt{3/2}\ (3\lambda_3+1)$ and $\eta= \lambda_1- \lambda_2+\ 3/2\ \lambda_3+1$

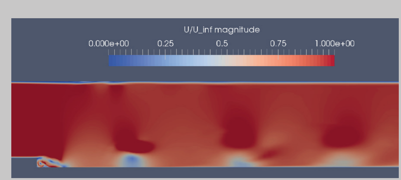
Training case (Re = 32k)

RANS



$q(x)_{train} = \{q_1, q_2, \ldots \ldots q_{10}\}$
$\tau_{RANS\_train}=\{\xi_{RANS\_train}, \eta_{RANS\_train}\}$

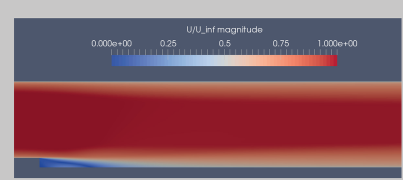
DNS



$\tau_{DNS\_train}=\{\xi_{DNS\_train}, \eta_{DNS\_train}\}$

Test case (Re = 36k)

RANS



$q(x)_{test} = \{q_1, q_2, \ldots \ldots q_{10}\}$
$\tau_{RANS\_test}=\{\xi_{RANS\_test}, \eta_{RANS\_test}\}$

DNS

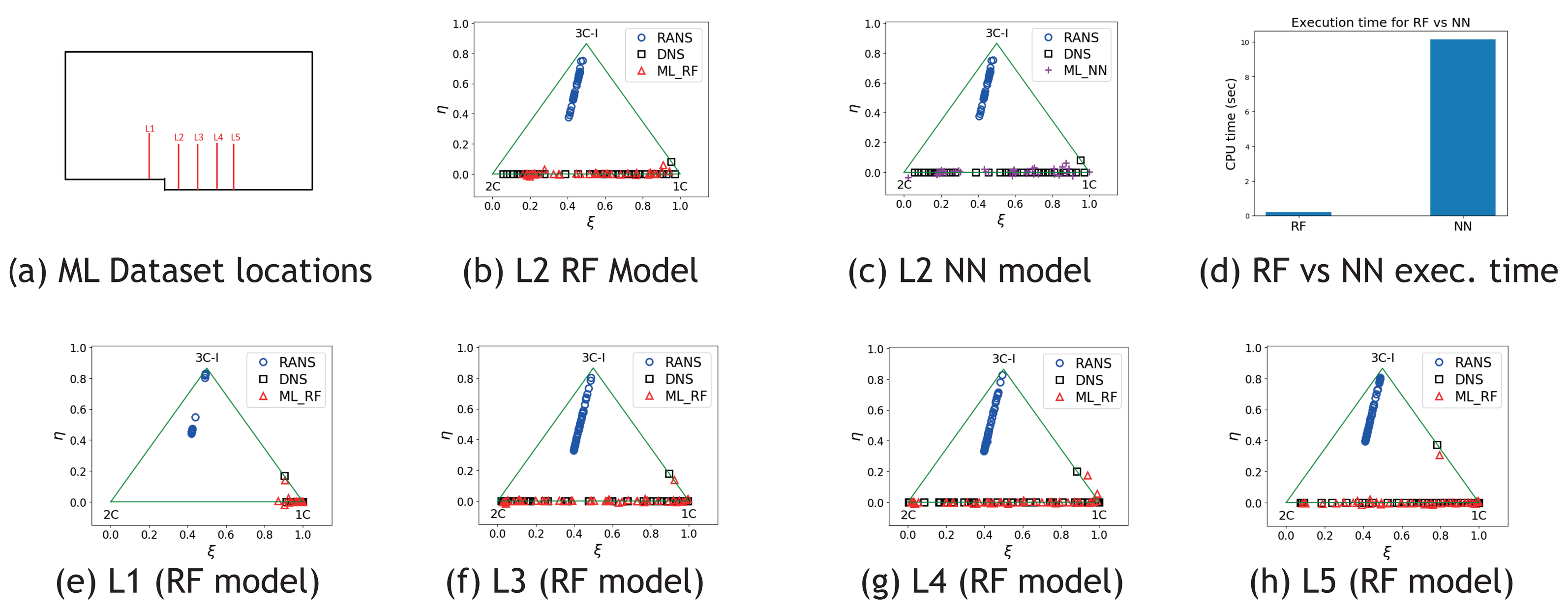
Not required once the model is trained

Table 1: Framework illustration

4. Results:

a. ML model Prediction results (1D):

The responses computed directly from RANS follow the typical plain strain rate assumption derived from Boussinesq hypothesis [1] whereas the ML predicted responses are along the line from vertex 1C to 2C states of turbulence. As observed in the figure 1(b) and 1(c), both RF and NN models provide similarly accurate results as DNS computation. All of them clearly show that the anisotropy pattern obtained, by k-ε based RANS model, along plain strain rate axis of barycentric representation is being corrected towards DNS resolved 1-component and 2-component states of turbulence. Since the training data is limited and only from one single simulation, there is a mismatch in magnitude of corrections which will be corrected as framework is improved further.

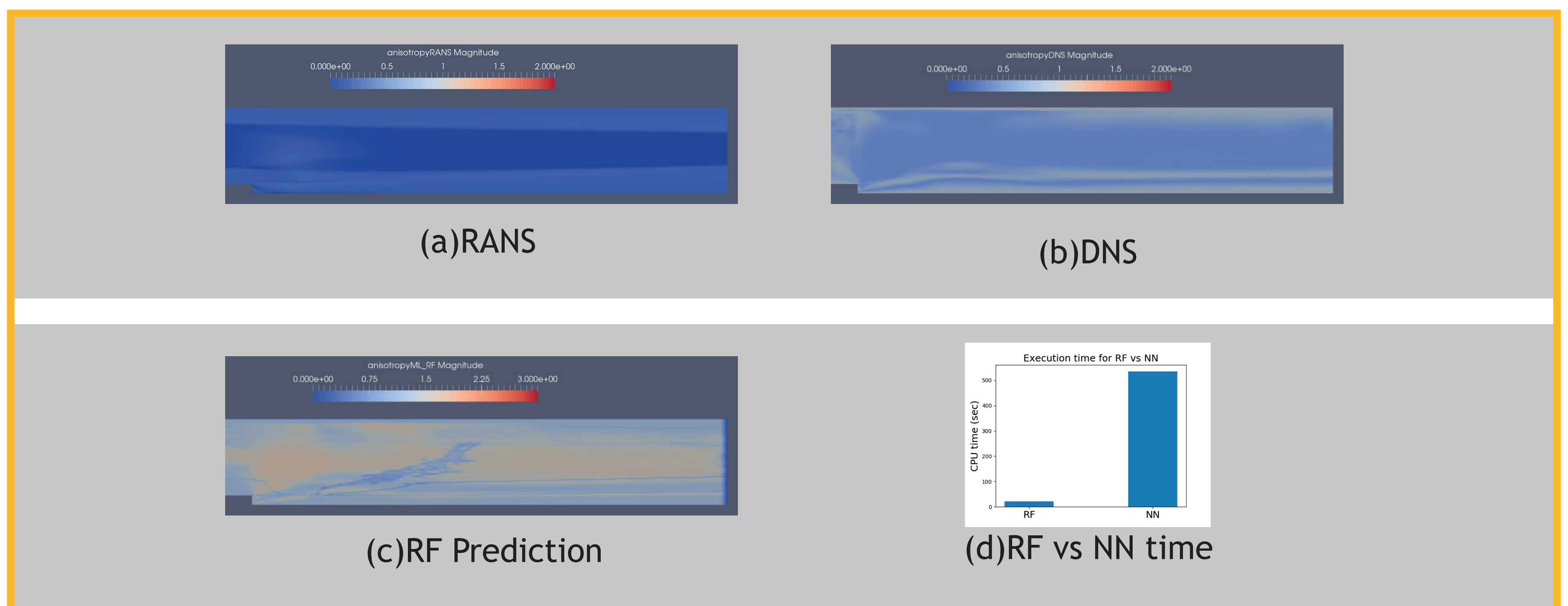


(a) ML Dataset locations (b) L2 RF Model (c) L2 NN model (d) RF vs NN exec. time
(e) L1 (RF model) (f) L3 (RF model) (g) L4 (RF model) (h) L5 (RF model)

Figure 1: Performance of ML model in 1D

b. ML model Prediction results (2D):

With the validation of 1D correction, the complete 2D flow domain information is fed to train ML models. The eigen value system corrected by the ML and RF algorithms is converted back to the anisotropic tensor (A), with eigen vectors uncorrected, and the 2D CFD domain of the test case is visualized in figure 2, by plotting magnitude of A computed using RANS, DNS and Random Forest approaches. As can be observed, the RANS predicted anisotropy is almost negligible in magnitude and even the qualitative similarity with DNS solution is very less. Whereas, the A tensor prediction by RF model is different in magnitude as compared to DNS solution but the prediction of A close to the bottom wall is more closer to DNS than RANS. It should be noted that correction of only eigen values and not vectors limits the capability of regression function constructed by machine learning models. Also, using 1 training simulation might not be sufficient for better predictions.



(a)RANS (b)DNS
(c)RF Prediction (d)RF vs NN time

Figure 2: Performance of ML model in 2D

5. Conclusions:

- The framework is established, through new function objects in OpenFOAM, to generate inputs and responses for training PIML model in 1D and 2D.
- The performance analysis of decision tree based Random forest and neural network ML models are done, in terms of accuracy and speed for 1D corrections. Though the accuracy is almost similar in Barycentric representations, NN based model requires more execution times in terms of CPU seconds. However, both approaches are to be included in the framework as the complexity of cases is going to increase.
- Currently, PIML model is used for correcting full scale 2D simulations. Although 2D predictions are only partially matching with DNS, the anisotropy prediction trend being closer to DNS than RANS is a positive aspect and by including eigen vector corrections for A tensor, it is expected to be similar to DNS.

6. Future work:

The further work includes incorporation of responses to correct eigenvector system in addition to the Eigen value based responses implemented currently. Also, the time series data of DNS simulation will be utilized using ML algorithms based on some form of customized Recurrent Neural Networks. The evaluation of possibilities is needed to be done to propagate the corrected Reynolds stress tensor to velocity flow field by also incorporating additional observations presented in Wu et.al[6]. The overall final objective of our work though is to improve the model further and validate its scope in practical automotive applications.

7. Acknowledgements:

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References

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