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Modelling of Equivariant Tensor Basis with Euclidean Turbulence Closure Neural Network

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ABSTRACT: Improved turbulence models are necessary for achieving more accurate solutions in Reynolds-averaged Navier-Stokes (RANS) simulations. RANS is widely used in various engineering applications, and enhancing its accuracy is crucial for geometry design and control applications. With the increasing availability of high-fidelity datasets, machine learning (ML) techniques offer the opportunity for data-driven inference of RANS equation closure terms. In accordance with Pope's theoretical analysis, ML turbulence closure models for RANS simulations are often used alongside feature engineering to provide an equivariant tensor basis. In this work, we replace this established approach by using Euclidean neural networks (e3nn). We design a bilinear architecture to equip the model with trainable tensorial operations, demonstrating that Pope's tensor basis is a special case of our model. We test the model on the Periodic Hills flow case dataset. Our approach significantly improves the prediction of anisotropic components of Reynolds stresses, leading to more accurate modelling of the flow field when integrated into RANS through single injection.

KEYWORDS: Fluid Dynamics, Turbulence, Machine Learning

1. Case Introduction

Modelling fluid flow often requires numerical methods due to the lack of a universal analytical solution to the Navier-Stokes equations. Direct methods that resolve all flow features need a fine computational mesh and many time-steps, which is not feasible for most engineering applications due to time constraints. This leads to the Reynolds-averaged Navier-Stokes (RANS) method, which models the influence of smaller vortices and solves the time-averaged flow field, incorporating closure models to account for turbulence. Most industrial simulations use eddy viscosity models for their ease of implementation and good performance [1], while Large Eddy Simulation (LES) is gaining attention for simpler cases despite requiring a finer computational grid and more time.

RANS simulation uncertainties fall into four categories [2]: information loss in Reynolds-averaging, representation uncertainties of Reynolds stress in mean fields, specific function selection, and parameter calibration of the turbulence model. The second uncertainty is focus in this study.

In RANS, the term $\tau_{ij} = -\overline{u_i' u_j'}$, called Reynolds stress, is like viscous stresses and represents the nonlinear convection term in the Navier-Stokes equation. Accurate modeling of the Reynolds stress tensor (RST) is crucial for effective turbulence modeling. Most modern RST models are based on the Boussinesq analogy and are known as linear eddy viscosity models (LEVM) [3]. The assumption is that the anisotropic part of RST changes similarly to the viscous stress tensor and can be expressed as a linear function of the local mean rate of strain S_{ij}:

$$\tau_{ij} + \frac{2k}{3}\delta_{ij} = 2\mu_t S_{ij}, \quad S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \tag{1}$$

where: $\tau_{ij} + \frac{2k}{3}\delta_{ij}$ is the anisotropy of Reynolds stress, $k = \frac{1}{2}\overline{u_i' u_i'} = -\frac{1}{2}\tau_{ii}$ is the turbulent kinetic energy, and μ_t is the turbulent viscosity.

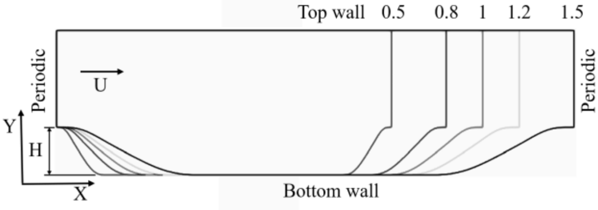

Fig. 1. Periodic hill cases visualization

Using high-fidelity data (DNS) to extract accurate RST is crucial for developing modern data-driven turbulence models. In this study the DNS data is periodic hill dataset from [4] with variable steepness of hill and constant Reynolds number equal to 5600. The visualization of case is shown in Fig 1. OpenFOAM [5] -v2312 with RST model [6] were used as numerical toolkits for all studies. The testing case is 1.2, the case 0.8 is a validation set used for model selection, and the remaining cases are used as training set

2. Machine Learning Setup

In this work, we seek a more general alternative to symbolic engineering of equivariant tensor basis, instead adopting Euclidean Neural Networks (e3nn) [7] to ensure equivariant behaviour of the neural model. To provide interactions between tensors of different ranks and parities, we construct a model of blocks that use separate linear layers to produce two representations and use the Tensor Product layer. As the magnitude of the input data has significant importance in machine learning physics, we use SiLU activation. In analogy to SiLU, we also apply sigmoid activation to one of the representations within the interaction block, while the other remains unchanged. We use simpler *uvu* Tensor Product layers within the interaction blocks and the Full Tensor Product for readout. The entire architecture is shown in Fig. 2. The latent dimension of our model is either "32x0e 32x1o + 32x1e + 32x2e": the network models scalars, vectors, pseudovectors, and (spherical, or equivalently, symmetric and traceless) rank-2 tensors; 32 variables of each of those kinds.

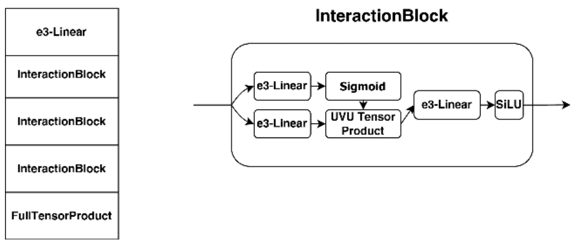

Fig. 2. Schematic architecture of e3-Turbulence model. Each interaction block has a Tensor Product layer that allows for combination of knowledge from variables that change differently under symmetric transformations

The output of predicted RST field is written in format of OpenFOAM field and single injected at the beginning of simulation. Training environment is based on PyTorch [8].

3. Prelimnary results

A comparison of the flow fields is shown in Fig. 3. The cases were considered converged when the residuals reached a level of 1×10^{-5}. The prediction of the Reynolds Stress Tensor (RST) field (R PRE) is sufficiently accurate to produce a similar velocity field in the test case. The agreement is better when comparing the velocity field in the X direction, leading to a global solution with good agreement with DNS, with an averaged absolute global error of approximately 0.5%. The recirculation region is slightly underpredicted due to weaker agreement of the velocity in the Y direction. The resultant injected R PRE differs from the original R DNS and significantly underestimates the turbulence intensity on the slope of the hill.

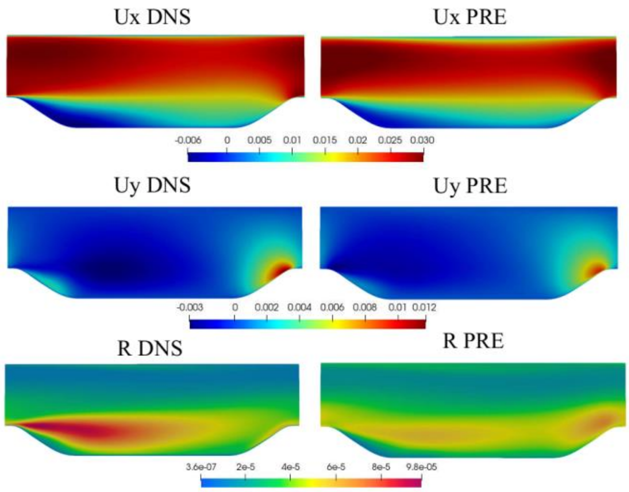

Fig. 3. Velocity field comparison of RANS simulation (R PRE) with time averaged DNS results with additional RST field comparison

4. Summary

Preliminary results indicate the potential to obtain useful data from the evaluated combination of Reynolds-Averaged Navier-Stokes (RANS) and machine learning (ML) techniques. The two most significant results are as follows:

1) There is an improvement in computational time, with approximately a 20% speed-up compared to the baseline RANS case, without improved Reynolds Stress Tensor (RST) in the 1.2 Periodic Hill test case.
2) The accuracy of the solution is comparable to baseline k-omega SST results, with discrepancies in the flow reattachment length being lower than 5%.

Further information will be obtained when the e3nn is tested on different test cases from wider datasets [9].

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