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Predicting Cases of Isotropy in Turbulence Modeling using Physics Informed Machine Learning

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Abstract

Turbulence is a well-ploughed area in computational fluid dynamics (CFD). However, modern DNS-LES-RANS techniques are still computationally heavy and/or inaccurate at high Reynolds numbers. Due to lack of fine-granularity and optimality with manual tuning of model parameters, an opportunity for machine learning emerges. This paper delivers accurate turbulence models dynamically, by combining decades old scientific turbulence foundations with novel Physics Informed Machine Learning (PIML) techniques. As a starting point, we train different regression and neural network algorithms over Isotropy Cases, yet we plan to extend our work with all anisotropy cases that can be represented within the universal Lumley triangle.

Keywords: physics informed machine learning, turbulence, anisotropy, neural networks, OpenFoam

1 Introduction

Turbulence has been one of the most important natural phenomena that impacts the accuracy of computational fluid models. Turbulence modelling becomes inevitably critical for most engineering problems of interest especially at high Reynolds numbers. Direct Numerical Simulations (DNS) that solve Navier-Stokes (NS) equations in its full form (time & space) are accurate, but computationally infeasible.

Reynolds Averaged Navier Stokes (RANS) methods address this problem by averaging all flow related parameters in the NS equations, thus saving serious amounts of computational load. However, RANS equations involve Reynolds stresses that cause the so-called “closure problem”.

In this paper, a generic framework for training anisotropy invariant (AI)-based [1, 2, 3] Reynolds Stress Models (RSM) is developed. The AI-model makes use of a constitutive relation between known and unknown tensors. The relations are weight functions of second (II) and third (III) invariants of the anisotropy tensor of Reynolds stresses (a_{ij}) and a turbulence Reynolds number ($\mathrm{Re}_{\lambda}^{*}$). These functions are constructed between the limiting states (1C-2C-3C) of turbulence as illustrated in the Lumley Anisotropy Triangle [4, 5] in Figure 1 where $\mathrm{Re}_{\lambda}^{*}$ ranges between zero to infinity ($\mathrm{Re}_{\lambda}^{*}$: 0→∞). This training framework is used to reduce the computational cost of turbulence modelling while preserving accuracy. In the case of determining the coefficients of this function, different Machine Learning (ML) methods are proposed.

As a starting point, this work considers the isotropic turbulence cases where the second and third AI are zero. Therefore, only the impact of turbulence Reynolds number, $\mathrm{Re}_{\lambda}^{*}$ needs to be included in the RSM model.

Physics Informed Machine Learning (PIML) or Physics Informed Neural Networks (PINNs) [6] utilize the learning power of NN by exploiting physical laws that govern the processes described by series of partial differential equations. We will initially focus on predicting parameters of the transport equation used by Jovanovic´et al. [1] as detailed in Section 2 (Methodology). While there are similar proposals for using ML in turbulence modelling, most attempts rely on either finding the parameters of k-ϵ method [7] or concentrate on limited turbulence problems [8]. We contribute to turbulence modelling by creating a constitutive equation-based [1] ML framework.

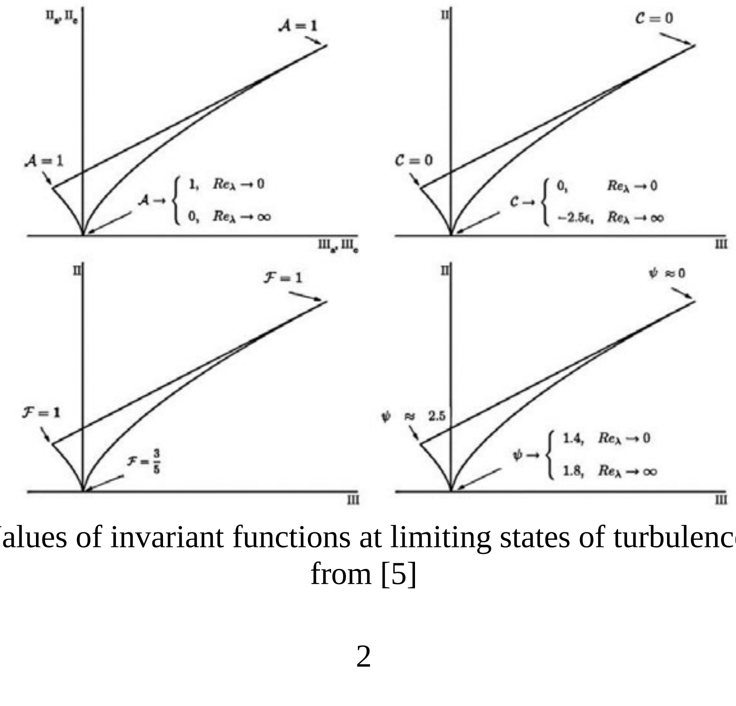

Figure 1: Values of invariant functions at limiting states of turbulence. Adapted from [5]

2 Methods

A Reynolds Stress Transport (RST) model is introduced by Jovanović *et al.* [1] that offers an alternative constitutive relation for finding Reynolds Stress term for homogeneous turbulence as:

$$\frac{\partial \overline{u_i u_j}}{\partial t} = P_{ij} + \mathcal{C} a_{ij} + a_{ij} P_{ss} + \mathcal{F}\left(\frac{1}{3} P_{ss} \delta_{ij} - P_{ij}\right) - 2\mathcal{A}\epsilon a_{ij} - \frac{2}{3}\epsilon \delta_{ij} \quad (1)$$

where $\mathcal{A}, \mathcal{C}, \mathcal{F}$ correspond to anisotropy invariant functions and $a_{ij} = (\overline{u_i u_j}/2k) - 1/3\delta_{ij}$ is the anisotropy tensor of the Reynolds stresses. These functions can be approximated by calculating their values on limiting states of turbulence with one or two components. When $\mathcal{A}$ is written in terms of its weighing functions, one obtains the following relation:

$$\mathcal{A} \cong \begin{cases} (1-J)\mathcal{A}_{1c} + J\mathcal{A}_{iso}, & III_a > 0 \\ (1-J)\mathcal{A}_{2c-iso} + J\mathcal{A}_{iso}, & III_a < 0 \end{cases} \quad (2)$$

Lumley [4] postulated that for limiting states of isotropy ($J=1$, $\mathcal{A}=\mathcal{A}_{iso}$) when turbulence has two components, the following relations can be written between III_a and II_a :

$$II_a = \frac{2}{9} + 2III_a \quad (3)$$

and for isotropic turbulence,

$$II_a = III_a = 0 \quad (4)$$

Using Equations 2, 3, 4 it can be shown that J equals to:

$$J = 1 - 9\left(\frac{1}{2} II_a - III_a\right) \quad (5)$$

Now that J is resolved in terms of invariant functions and limits are set, a new weighting function for finding $\mathcal{A}$ must be set. According to [1], $\mathcal{A}$ can be written as:

$$\mathcal{A} \to (1-\mathcal{W})\mathcal{A}_{Re_\lambda^* \to \infty} + \mathcal{W}\mathcal{A}_{Re_\lambda^* \to 0} \quad (6)$$

where Re_λ^* is a function of q (RMS of velocity fluctuation), λ_g (dissipation length) and ν (viscosity):

$$Re_\lambda^* = \frac{q\lambda_g}{\nu} \quad (7)$$

Jovanović [1] represented the ratio of λ_g to L_g (integral length) as a carefully tuned function of Re_λ^*:

$$\frac{\lambda_g}{L_g} = -0.049Re_\lambda^* + \frac{1}{2}\left(0.009604Re_\lambda^{*2} + 10.208\right)^{\frac{1}{2}} \quad (8)$$

Equation 8 results in 0 when $Re_\lambda^* \to \infty$ and 1.597 when $Re_\lambda^* \to 0$. Therefore, $\mathcal{W}$ can be represented as,

$$\mathcal{W} = \frac{\lambda_g}{1.597L_g} \quad (9)$$

Which is illustrated in Figure 2. Note that we skip the details for obtaining $\mathcal{C}, \mathcal{F}$ here for brevity and refer the readers to [1] for details.

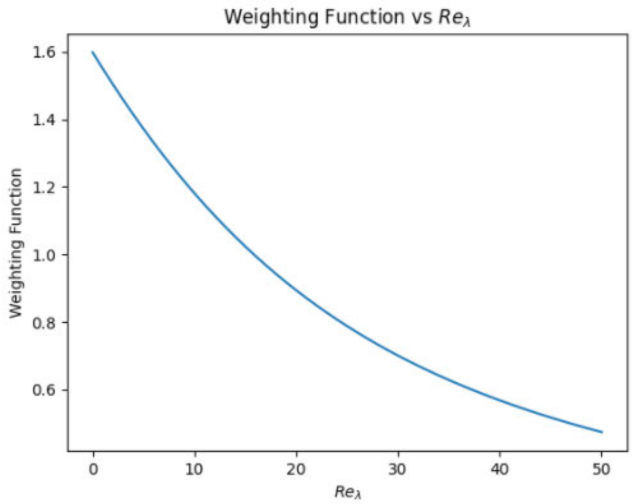

Figure 2: The relation between Weighting function and Re_λ^* in [1].

In this paper, we aim to accurately predict the $\frac{\lambda_g}{L_g}$ ratio using PIML to find the coefficients denoted in Equation 1 as follows:

1- For different Re_λ^* (0→50)
2- Obtain $\frac{\lambda_g}{L_g}$ from DNS data for forced isotropic cases
3- Use the selected ML algorithm to train with DNS data
4- Obtain a new model by predicting a new relation for $\frac{\lambda_g}{L_g}$ and Re_λ^*
5- Confirm RST model by using decaying isotropic cases.

3 Results

We currently present data for one isotropic forced turbulence case here. Using OpenFoam CFD software, models with different granularities are prepared (e.g. 64x64x64) for periodic boundary conditions and DNS results for velocity and Reynolds stresses over time (e.g. t=60 seconds and step=0.001 seconds) were gathered. Probes with different coordinates are placed in x-y-z axes. Figure 3 depicts the meshed domain of analyses. For testing the validity of the turbulence, evolution of anisotropy tensor components (a_{ii}) of the data taken from the center of the solution domain over time are plotted (Figure 4). They converge to zero (0) as it is supposed for isotropic turbulence. Figure 5 is the energy spectrum of the turbulence data which is compliant with Kolmogorov's (-5/3) power law. Dissipation of turbulence to viscosity at the end can also be observable via this graph. In our full paper, we will be presenting results from more isotropic turbulence cases with higher-granularity and longer times. Purpose of these experiments are to obtain the verified DNS results of Table 1 in (Eswaran & Pope) [10] for machine learning models. This way we will first complete steps 1-2 in our methodology followed by steps 3-4-5 for PIML modelling of turbulence.

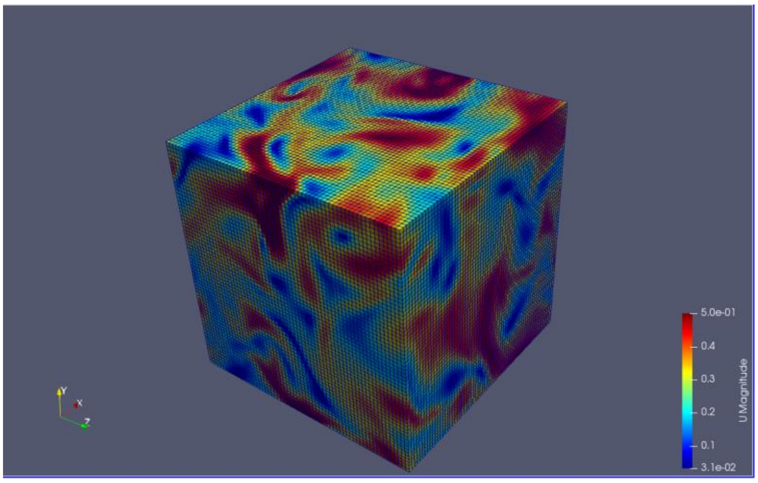

Figure 3: 64x64x64 mesh and view of velocity component in forced box simulation.

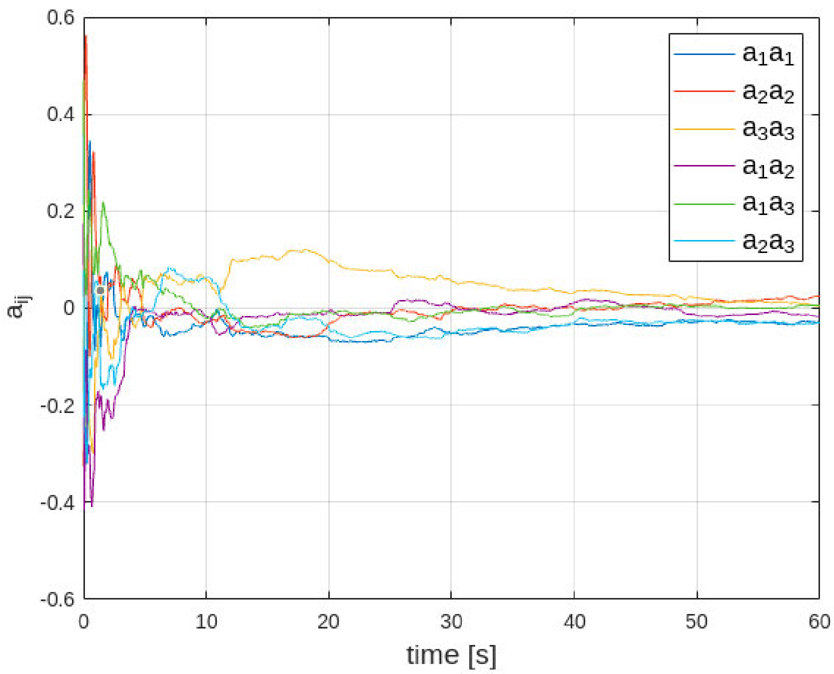

Figure 4: Change of diagonal components of the anisotropy tensor over time

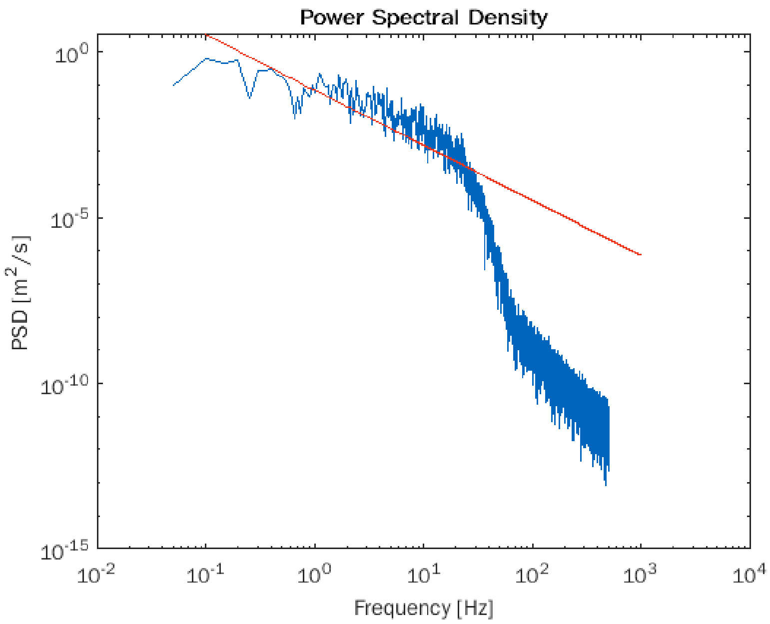

Figure 5: Log-log scale for power spectrum density (PSD) and redline illustrating Kolmogorov slope of (-5/3). After this region the turbulence dissipates.

4 Conclusions and Contributions

This work aims to deliver accurate turbulence models by combining anisotropy invariant (AI)-based Reynolds Stress Models (RSM) with Physics Informed Machine Learning (PIML). We started obtaining DNS data for isotropy cases using OpenFoam CFD software and we will train different ML algorithms over these data in the future. We plan to extend our work with all anisotropy cases that can be represented within the universal Lumley triangle.

References

[1] Jovanovic´, J., Otic´, I., Bradshaw, P. “On the Anisotropy of Axisymmetric Strained Turbulence in the Dissipation Range”. Journal of Fluids Engineering, 125(3), 401–413, 2003, doi:10.1115/1.1568355

[2] Banerjee, S., Krahl, R., Durst, F., Zenger, C. “Presentation of anisotropy properties of turbulence, invariants versus eigenvalue approaches”. Journal of Turbulence, (8), N32, 2007, doi:10.1080/14685240701506896

[3] Banerjee, S, Ertunç, Ö., Durst, F. “Measurement and modeling of homogeneous axisymmetric turbulence”. Journal of Turbulence, (10), 2009, doi:10.1080/14685240902744692

[4] Lumley, J. L., Newman, G. R. “The return to isotropy of homogeneous turbulence”. Journal of Fluid Mechanics, *82*(1), 161–178, 1977, doi:10.1017/s0022112077000585

[5] Ertunc, Ö. “Experimental and numerical investigations of axisymmetric turbulence. PhD Dissertation, Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg, 2007.

[6] Raissi, M., Perdikaris, P., Karniadakis, G. E. “Physics-informed Neural Networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations”. Journal of Computational Physics, 378, 686–707, 2019, doi:10.1016/j.jcp.2018.10.045
[7] Luo, S., Vellakal, M., Koric, S., Kindratenko, V., Cui, J. “Parameter identification of RANS turbulence model using physics-embedded neural network”. Lecture Notes in Computer Science, 137–149, 2020, doi:10.1007/978-3-030-59851-8
[8] Kaandorp, M. L., Dwight, R. P. “Data-driven modelling of the Reynolds stress tensor using random forests with invariance”. Computers & Fluids, 2020, 104497, 2020, doi:10.1016/j.compfluid.2020.104497
[9] Wu, J., Xiao, H., Sun, R., Wang, Q/ “Reynolds-averaged Navier–stokes equations with explicit data-driven Reynolds stress closure can be ill-conditioned”. Journal of Fluid Mechanics, 869, 553–586, 2019, doi:10.1017/jfm.2019.205
[10] Eswaran, V., Pope, S. B. “An examination of forcing in direct numerical simulations of turbulence”. Computers & Fluids, 16(3), 257–278, 1988, doi:10.1016/0045-7930(88)90013-8