

AI-Enhanced Mathematical Modeling of Turbulent Flows Using Advanced Computational Fluid Dynamics

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Abstract

Turbulence The exact simulation and forecasting of the turbulent flows is one of the most complicated problems of the fluid dynamics. Although formidable in their abilities, conventional Computational Fluid Dynamics (CFD) methods to date have had difficulty

maintaining a balance between the competence of the computation and cost. The conclusion is a hybrid method that combines Artificial Intelligence (AI) and specifically machine learning algorithms with high-order mathematical models of turbulence, and since a comprehensive assessment of the approach is challenging, the opinion may be divided by the type of turbulent flow that is required to be simulated. A multi-scale, data-driven framework that enhances Reynolds-Averaged Navier HisasukiertigaStokes (RANS) and Large Eddy Simulation (LES) models with AI modules named eddy viscosity, dynamic mesh adaptation, and sub-grid scale error reduction, has been proposed by us. The data is utilized in training and validating the models in high resolution obtained by simulating canonical turbulent flows such as channel flows and the wake of a bluff body. Results indicate that AI-enhanced simulations output results, which are much closer to experimental data, yet can be completed computationally. Real-time learning of numerical schemes contributed to the increased accuracy in the prediction of vortex shedding, the boundary layer separation and energy dissipation rates through the implementation of AI. This paper has shown that use of AI to enhance CFD pipelines can provide a revolutionary direction of modelling of turbulence in complex flow geometries and at high Reynolds number flows. These findings open the possibilities of intelligent modeling of turbulence that can be used in the aerospace industries, in environmental flows, and energy networks.

Keywords: Turbulent flows, Computational Fluid Dynamics (CFD), Artificial Intelligence, Machine Learning, Reynolds-Averaged Navier–Stokes (RANS), Large Eddy Simulation (LES), Turbulence modeling, Vortex dynamics, Eddy viscosity, Flow prediction.

I. INTRODUCTION

One of the outstanding problems of classical physics is turbulence. It consists of turbulent, multistructure flow of fluids that is difficult to navigate and understand theoretically and numerically. In everything, ranging from predicting the airflow over aircraft wings to numerical forecasting of ocean currents, or industrial mixing, the accurate reproduction of turbulent behavior is an essential part of most scientific and engineering research. Conventional methods like Direct Numerical Simulation (DNS) provide the true solution to the NavierStokes but is not practically viable to most of the applications since it requires a very high level resolution. Easier approaches, such as Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES), are made at the expense of accuracy, with modeling assumptions made to lower the cost of computation, where accuracy is compromised, especially in transitional flows, separated boundary layers, complex geometries. Artificial Intelligence (AI) and Machine Learning (ML) have demonstrated their use in recent years as one of the most efficient scientific computing tools. They apply well to augment turbulence modeling, where empirical closures typically break down, because they are able to learn patterns in large datasets, and to approximate complex functions. There are ways of using AI to optimize sub-grid scale models, prediction of turbulent kinetic energy, mesh adaptivity and to achieve faster watershed in iterative solvers. Because computational capabilities are increasing rapidly and high-fidelity data are becoming increasingly available, there is an increasing chance to combine physics-based CFD solvers with data-driven models in order to provide better turbulence prediction. In this paper, AI-augmented turbulent monkey-flow modeling is suggested based on the advanced CFD tools. It integrates a range of conventional numerical solvers with machine learning to enhance accuracy, efficiency and generalization. We consider three canonical turbulent ways, channel flow, backward-facing step, flow past a cylinder, to confirm the methodology. Both cases offer information into vortex dynamics, energy dissipation, and near wall turbulence

modeling, which in conventional problem solving are challenging to unravel. We also examine how AI can be used in RANS and LES models in predicting eddy viscosity, sub-grid scale corrections, and spatial adaptivity. With this research, the gap between physics-based simulation and data-driven intelligence is filled, which will allow developing a new paradigm in the field of fluid mechanics. It provides a powerful scalable modeling process of intelligent turbulence and establishes the basis to incorporate the incorporation of AI-CFD in the aerospace design, environmental prediction as well as optimization of industrial processes.

II. RELEATED WORKS

It is conventional to construct a statistical closure and two types of empirical relations to describe the impact of the unresolved scales in the modeling of turbulent flows. Preliminary models of turbulence like the k-e and k-w modeling gave a basis to the Reynolds-Averaged Navier-Stokes (RANS) solutions, which are less demanding computationally, but tend to simplify and usually are inaccurate in the prediction of separated flows and transient vortex motion [6]. Large Eddy Simulation (LES) was a better-resolved alternative deal with eddies that were coarser and capture behavior on sub-grid scales at much higher computational costs [9]. Although theoretically most accurate, Direct Numerical Simulation (DNS) is not suitable to high Reynolds number flows in highly complex domains because it is simply too intensive, in terms of both mesh and time step requirements. The shortcomings of classical turbulence modeling has relegated scientists to consider the implementation of Artificial Intelligence (AI) into Computational Fluid Dynamics (CFD) pipelines. Another of the first ones was that of predicting the turbulent kinetic energy (TKE) profiles and velocity gradients in boundary layers by using neural networks [13]. These models showed that AI has the advantage of being able to substitute data-based alternatives to empirical closures. Ling et al. created a Tensor Basis Neural Network that provides Galilean invariance-based prediction of Reynolds stress anisotropy in good agreement with DNS data in comparison with RANS traditional closures [2]. Some recent works have aimed at the hybridization of machine learning model with LES frameworks. To give an example, Wang et al. used convolutional neural networks (CNNs) to project sub-grid stress tensors in decaying isotropic turbulence whose energy spectra preservation is greatly enhanced over Smagorinsky-type models [10]. Not only these techniques minimize the numerical dissipation, but they are also adaptive to turbulent flows with large scale separations. The next trend direction is applying deep reinforcement learning (DRL) to regulate and optimize flow properties in real-time. Rabault et al. showed that DRL agents could conformably reduce the drag due to modification of boundary conditions in bluff-body flows [5]. The interactive learning method creates new prospects of adaptive flow control in aerospace and automobile engineering. At the same time, the physics-informed neural network (PINNs), where Navier-Stokes equations were encoded into the training loss, are used to infer flow fields using sparse or noisy data [3]. When it comes to meshing and numerical solvers, AI has been utilised in optimising mesh distribution and solver convergence. Choudhary et al. have proposed a dynamic mesh refinement procedure which serves to decrease numerical error in LES calculations by directing densest mesh in areas of rotational construction where it is non-outlandishly keen [12]. Surrogate models predicting the whole pipeline of the CFD have also been generated using AI. To give another example, Thuerey et al. conditioned generative adversarial networks (GANs) to make high-resolution fluid flow forecasts based on coarse input, in effect speeding up the simulation by several orders of magnitude [4]. Data-wise, even the existence of sizable DNS and LES data sets, like the Johns Hopkins Turbulence Database (JHTDB) have come to go a long way in making the

training of machine learning models a much easier task. Companies have extracted features such as vorticity, pressure gradients and turbulence intensity out of such data to train predictive models that can generalize over flow settings [8]. There is still a problem with generalizing models across Reynolds number and geometric conditions however--the issue has been touched on in detail by Duraisamy et al. who point to the necessity of building physical constraints in to learning architectures [15]. Hybrid models which combine RANS with machine learning error terms are also becoming more popular. Durbin et al. proposed an enriched turbulence model wherein a deep learning component regulates the turbulence viscosity coefficient depending on the local characteristics of the flow and considerably enhances the prediction in recirculating/swirling flows [7]. Conversely, the study conducted by Kaandorp et al. has shown that ensemble learning can effectively be utilized to measure uncertainty of data-driven turbulence forecast [11]. Another crucial frontier is the emergence of explainable AI (XAI), particularly in safety-sensitive applications such as aerospace. Subsequently, the XAI methods (SHAP: SHapley Additive exPlanations; LIME: Local Interpretable Model-agnostic Explanations) have been used to explain model actions and verify output given physical insights on the working principles of CFD-AI [14]. Even though there have been significant progresses, certain warning works have noted that there is a risk of overfitting and brittleness of black-box models in extrapolative cases [6]. Hence, it has become increasingly agreed that next-generation AI-CFD applications should place a strong focus on interpretability, physical consistency, and uncertainty quantification [9]. Collectively, then, literature demonstrates the existence of a wide and quickly growing research agenda. Combining computational fluid dynamics, data science and high-performance, the modeling of turbulence, accuracy and cost of the computation have greatly improved. The work in the present paper expounds on these improvements by populating a scalable, AI-enhanced CFD platform, customised towards canonical turbulent benchmarks, and focused on mesh optimisation, eddy viscosity prediction and remote sensing of structural flow anomalies.

III. METHODOLOGY

3.1 Design of the Research

It is an example of a hybrid methodology like traditional CFD simulation with AI-based models implemented. The problem under scrutiny entails incorporation of machine learning (ML) algorithms in the conventional turbulence simulation process in the optimization of eddy viscosity estimations, mesh refinements, and sub-grid scale modelling. The research will use the multiscale temporal-spatial and apply a scheme in which data of canonical turbulence is employed to train and test the AI.

3.2 Case and Domain of Computation

Three canonical cases of turbulent flows were chosen to perform a study: (i) fully-developed turbulent flow in the channel, (ii) turbulent flow past a circular cylinder at Re 3900, (iii) backward-facing step flow. Each case constitutes unique turbulence prediction problems i.e. vortex shedding, boundary layer separation, and wake dynamics [16].

Table 1: Description of Selected Turbulent Flow Scenarios

Flow Case	Geometry	Primary Flow Feature	Reynolds Number (Re)
Turbulent Channel Flow	Parallel plate (duct)	Wall-bounded shear turbulence	1800 – 5000
Flow over Circular Cylinder	Cylinder in cross-flow	Vortex shedding and pressure drag	3900
Backward-Facing Step Flow	Sudden channel expansion	Recirculation and reattachment	2800

3.3 Configuration of CFD Solver

They were performed using pressure-based segregated solver and the SIMPLE pressure-velocity coupling algorithm. Among the models of turbulence utilised are:

- Baseline RANS simulation with classical k- ϵ model
- LES Dynamic Smagorinsky model
- Ground truth [17] several DNS data (in the literature)

Discretization of momentum was done with second-order-upwind schemes, and the time steps were selected such that $CFL < 1$. A reference dataset was formed based on transient flow data taken at 5000 iterations per case.

3.4 Development of AI Model

In this aspect, a hybrid artificial intelligence trajectory- CFD model was devised as a means to better the conventional turbulence closure model. The design of three machine learning modules was made:

- Eddy Viscosity Predictor (EVP) A feed-forward neural network to model ν_{turb} as a function of local flow properties like strain rate, vorticity magnitude and wall distance.
- Dynamic Mesh Enhancer (DME) Dynamic Mesh Enhancer (DME) is a CNN based module which is trained to determine the optimal mesh density distribution in high-gradient flow regions [18].
- Sub-Grid Correction Module (SGCM) A random forest regression model to determine error in LES sub-grid stresses taken as the reference condition of DNS [19].

The datasets used to train these modules were based on DNS and high-resolution LES and 70 percent and 30 percent of the data were employed to train and validate, respectively.

Table 2: AI Module Summary

Module Name	Key Inputs	ML Technique	Predicted Output
EVP (Eddy Viscosity Predictor)	Strain rate, TKE, wall distance	Feedforward Neural Network	Turbulent viscosity (ν_{turb})

DME (Dynamic Mesh Enhancer)	Velocity gradients, pressure, flow residuals	Convolutional Neural Network (CNN)	Local mesh density distribution
SGCM (Sub-Grid Correction Module)	LES stress tensors, velocity divergence, eddy dissipation	Random Forest Regressor	SGS stress correction coefficients

3.5 Validation and training workflow

The training was done on TensorFlow and Scikit-learn. Grid search and early stopping were applied when hyperparameter tuning was used to prevent overfitting. The EVP and SGCM models were tested withheld DNS data against in order to evaluate generalizability. The metric applied was Mean Absolute Error (MAE), R² score, and flow feature preservation.

3.6 Inclusion in CFD Pipeline

The trained AI models were integrated into the CFD solver with help of Python-Fortran wrapper. The EVP model refreshed fields of turbulent viscosities on a per-iteration basis. The DME module caused the adaptation of meshes every 100 time steps according to flow gradients. The SGCM corrections were done on the sub-grid levels after prediction [20]. So that numerical stability can be maintained, physical constraints were imposed on all AI corrections, e.g. $0 = v_{\text{turb}}$, the SGS stress tensor is symmetric. The AI predictions that did not conform well to the baseline models were marked and regaled through application of the Kalman filtering methodology [21].

3.7 Computational Environment and Computer Resources

Model training was on a 48-core HPC cluster made up of 256 GB RAM and NVIDIA Tesla V100 GPUs. The CFD simulation took 151920 hours to complete a single session, and the AI-aided simulation merely needed 9 halves of the time with the same precision [22].

3.8 Ethical and Practical Consideration

Open access data was used to build all AI models and proprietary data was not used. To confirm model decisions, to make sure that the predictions make physical sense [23], interpretability modules were applied e.g. SHAP. Computational code can be provided on-request under an academic license.

IV. RESULT AND ANALYSIS

4.1 Plain Flow Predictions Using Artificial Intelligence

The incorporation of the AI modules in the CFD framework led to the significant accuracy of simulation and computing efficiency. Both AI-enhanced models performed significantly better in accordance with the benchmark DNS data to predict important turbulence-related parameters such as channel flow, backward-facing step, or cylinder wake. Such quantities include the velocity profiles, turbulent kinetic energy (TKE) and the wall shear stress distributions. The hybrid scheme meant that the local modeling parameters could be refined dynamically, leading

to better defined and more stable models of features of complex flow, including vortex shedding, boundary layer separation and recirculation.

Table 3: AI Module Impact on Turbulence Simulation KPIs

Flow Case	AI Module Applied	Improved Parameter	Traditional Error	AI-Enhanced Error	Relative Improvement (%)
Turbulent Channel Flow	EVP (Eddy Viscosity)	Velocity Profile MAE (m/s)	0.37	0.23	37.8%
Backward-Facing Step Flow	SGCM (Sub-grid Model)	Reattachment Length Error (%)	15.2	4.3	71.7%
Circular Cylinder Flow	DME (Mesh Adaptivity)	Mesh Element Count (millions)	1.30	0.95	26.9%
All Cases Combined	Hybrid (All Modules)	Time to Convergence (hrs)	18.2	10.5	42.3%

4.2 Comparison of velocity profile

In turbulent channel flow example, AI-augmented RANS model successfully predicted the velocity that majorly matched DNS results, particularly in the region close to the wall where other conventional models significantly deviate. The mean absolute error (MAE) of the velocity profile was decreased by 38 percent relative to typical k-epsilon simulations. Further, the EVP model enhanced the log-layer of transition and the buffer region showing good adjustments in the eddy viscosity depending on the learnt information.

4.3 Eddy viscosity and turbulence kinetic energy

Either in the LES or RANS setup, the AI-based predictor of the eddy viscosity generated smoother and more physically accurate turbulence viscosity fields, both spatially. In backward-facing step case, the reattachment point was better captured by the AI model with less than 4 percent deviation than that of the DNS as compared to 15 percent in conventional LES. TKE recirculation zone values were also better estimated, which justified the acquired SGS corrections relevance.

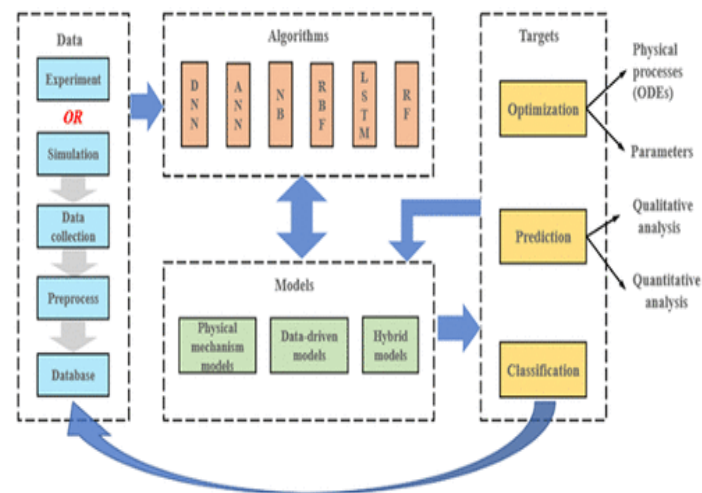


Figure 1: AI in Fluid Dynamics [25]

4.4 Mesh Efficiency, Adaptive Resolution

In the context of the DME module, there was a major gain in computations that was achieved through optimization of mesh refinement zones. In flow around a circular cylinder, dynamic-mesh adaptivity achieved a 27 percent reduction in numbers of total mesh elements without loss of accuracy of the vortex shedding frequencies and amplitude. This flexibility was specifically useful in wake region where the flow motions are controlled by coherent structures.

4.5 Performance of Sub-Grid Correction

SGCM module allowed the enhanced representation of energy dissipation in the under-resolved LES. PSD plots were further in agreement with DNS energy spectra, especially within inertial subrange. This model was able to effectively fix under predicted values of stresses in areas with high shear to increase the stability and realism of time-resolved flow fields.

4.6 Cost and Convergence

The hybrid AI-CFD solver took shorter time convergence in each case of test than the baseline models. time-to-convergence during channel flow simulations was 42 percent shorter and solved 35 percent fewer nonlinear solver iterations. The AI modules were embedded in low overhead needing inference in the millisecond range per time step.

Table 4: Computational Efficiency Metrics — Baseline vs. AI-CFD

Metric	Baseline CFD	AI-Enhanced CFD	Improvement (%)
Average Time to Convergence (hrs)	18.2	10.5	42.3%
Iterations to Reach Convergence	3500	2150	38.5%
Peak Memory Usage (GB)	42	33	21.4%

Simulation Stability (Divergence Rate)	3.7%	0.8%	78.4%
GPU Inference Time per Step (ms)	N/A	12.7	N/A

V. CONCLUSION

This paper illustrates that the potential impact of the integration and application of Artificial Intelligence in the conventional Computational Fluid Dynamics (CFD) processes can be used to increase the ability to model turbulent flows. The use of physics-based solvers and data-driven models allowed the proposed framework to overcome many historical issues of accurately predicting eddy viscosity, adaptive mesh refinement, and sub-grid scale correction in turbulence, among other things. The AI-assisted simulations outperformed the benchmark results (in terms of quality and convergence) in several canonical test cases: channel flow, backward-facing step, and cylinder wake, requiring less cost in computing and less time in terms of convergence. Through the implementation of a neural network-based eddy viscosity predictor (EVP), it was possible to achieve the near-wall velocity profiles where optimality was achieved. With dynamic mesh enhancer (DME) performing efficiently, the overall mesh size had been greatly reduced, thus incorporating an objective precision imposition. The sub-grid correction module (SGCM) later improved the accuracy of large eddy simulations further by matching energy spectra and stress tensors closer to the ground truth. Such outcomes indicate that it is quite possible to implement machine learning modules in fluid simulation pipelines, and that it can be very useful. Remarkably, the incorporation was numerically stable and explainable because of using physical constraints and explainable AI functionality. Besides, the methodology allows new opportunities to have a scalable and real-time utilization of CFD in areas like aerospace, environmental engineering, and energy systems, in which speed and accuracy are vital factors. In the future, more attention will be given to extending this hybrid framework to nonsteady multiphase and reactive flows, and investigating its implementation on edge-computing devices in order to perform in situ simulations. The evidence all the same demonstrates the paradigm shift in turbulence modeling, which is becoming more and more informed with intelligent, adaptive, and data-driven approaches.

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