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ENHANCING LES TURBULENCE MODEL IN COMPUTATIONAL FLUID DYNAMICS USING DEEP LEARNING

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ABSTRACT

Computational Fluid Dynamics (CFD) faces challenges in accurately modeling turbulent flows using traditional turbulence models. This paper presents a novel approach to improve Large Eddy Simulation (LES) turbulence modeling in CFD through deep learning. By training a deep learning model on a large dataset of high-fidelity turbulence simulations, intricate turbulence characteristics can be captured. Extensive numerical experiments on benchmark test cases and practical engineering problems demonstrate the superior predictive capabilities of the deep learning-enhanced turbulence models. They accurately capture critical flow features such as vortex shedding and boundary layer transition. Moreover, the deep learning models offer computational efficiency gains, enabling real-time simulations and optimization studies. This research paper highlights the potential of deep learning techniques to advance turbulence modeling in CFD, leading to more accurate and efficient computational tools for analyzing and optimizing turbulent flows in engineering systems.

Keywords: Turbulence, CFD, Deep Learning, LES, Turbulence Modeling, Model training

1. INTRODUCTION

Computational Fluid Dynamics (CFD) has revolutionized the field of fluid dynamics by providing a numerical approach to simulate and analyze complex flow phenomena in various engineering applications. Turbulent flows, characterized by their intricate vortical structures and chaotic nature, are encountered in numerous practical scenarios, ranging from aerospace design to environmental analysis. Accurate modeling of turbulence is crucial for understanding flow behavior, optimizing designs, and predicting performance. Large Eddy Simulation (LES) has emerged as a promising approach for capturing the energy-containing large-scale turbulent structures while modeling the smaller, unresolved scales. However, despite its advantages, LES still faces challenges in accurately predicting small-scale turbulence, which plays a vital role in many engineering processes. One promising avenue for improving turbulence modeling lies in the realm of deep learning. Deep learning algorithms have demonstrated remarkable success in diverse fields, such as image recognition, natural language processing, and pattern recognition. Leveraging these techniques in CFD can potentially overcome the limitations of traditional turbulence models and provide a data-driven approach to enhance LES predictions. By training deep learning models on high-resolution simulation data, it becomes possible to uncover complex correlations and patterns that may have been overlooked by conventional modeling approaches. This research aims to harness the power of deep learning techniques to enhance LES turbulence models, leading to more accurate and reliable predictions of turbulent flows in CFD simulations. For CFD simulation (i.e. pre-processing, meshing & simulation running) the OpenFOAM software v2012 is used and for post-processing ParaView software v5.8.0 is used. For deep learning algorithms the language used is Python in Google Colab.

1.1. Motivation

The motivation for this research paper on enhancing LES turbulence models in CFD simulation through deep learning can be summarized as follows:

1. To address the limitations of existing LES turbulence models and seek novel approaches to enhance their predictive capabilities.

2. To explore deep learning techniques as a potential solution to improve the accuracy and reliability of LES turbulence models.

3. Potential of deep learning: Deep learning has shown remarkable success in various fields, including image recognition, natural language processing, and pattern recognition. Leveraging the power of deep learning in the field of CFD and turbulence modeling presents an exciting opportunity to enhance the predictive capabilities of LES models.

4. Practical Applications: The research aims to have practical implications for industrial applications. Enhanced LES turbulence models can lead to more accurate predictions of flow behavior, which is crucial for optimizing designs, improving performance, and reducing costs in various engineering applications.

Overall, the motivation behind this research paper is to explore the potential of deep learning techniques to overcome the limitations of LES turbulence models and advance the field of turbulence modeling in CFD simulations.

2. LITERATURE REVIEW

2.1. LES Turbulence Modeling in CFD

LES (Large Eddy Simulation) turbulence modeling is a widely used approach in Computational Fluid Dynamics (CFD) for simulating turbulent flows. It is based on the concept of decomposing the flow field into large-scale turbulent structures, known as the resolved scales, and small-scale turbulent structures, known as the subgrid scales. In LES, the large-scale structures are directly resolved, while the small-scale structures are modeled using subgrid-scale models or closures. The resolved scales capture the dominant turbulent structures, which are responsible for energy transfer and overall flow behavior, while the subgrid scales represent the finer details of the turbulence that cannot be resolved due to computational limitations. LES offers several advantages over other turbulence modeling approaches, such as Reynolds-Averaged Navier-Stokes (RANS) modeling. It provides more accurate predictions of turbulence compared to RANS models by explicitly resolving large-scale structures, thereby capturing important flow features. Additionally, LES can handle complex flows and is well-suited for studying unsteady and highly turbulent flows.

LES turbulence modeling in CFD is based on the governing equations of fluid flow, namely the Navier-Stokes equations, with an additional subgrid-scale (SGS) model to account for the unresolved small-scale turbulence. The LES equations can be written as follows:

Conservation of Mass:

$$\nabla \cdot (\rho u) = 0$$

(2.1.1)

Conservation of Momentum:

$$\frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho u u) = -\nabla p + \mu \nabla^2 u + \tau_{SGS}$$

(2.1.2)

Conservation of Energy (for incompressible flows):

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho u E + \rho u) = -\nabla \cdot (k \nabla T) + \tau_{SGS} \cdot u + Q$$

(2.1.3)

The subgrid-scale model, τSGS, is an approximation that accounts for the unresolved small-scale turbulence. Various SGS models have been developed, such as the Smagorinsky model, dynamic models, and mixed models. These models aim to capture the effects of the small-scale turbulence on the resolved scales by estimating the subgrid-scale stress tensor, τSGS, based on the resolved flow variables.

$$\tau_{SGS} = -2\nu T S$$

(2.1.4)

where,

$$\nu T = (C_S \Delta)^2 |S|$$

(2.1.5)

$$S = \frac{1}{2}(\nabla u + (\nabla u)^T)$$

(2.1.6)

where,

-νT is the turbulent eddy viscosity

-S is the resolved strain-rate tensor

-C_S is the Smagorinsky constant (typically set to 0.1)

-Δ is the grid spacing (or filter width)

-$|S|$ is the magnitude of the resolved strain-rate tensor (S)

The turbulent eddy viscosity, νT, represents the effective viscosity that accounts for the turbulent mixing and energy transfer across the unresolved scales. It is related to the resolved flow variables and is typically modeled based on the local flow characteristics. The resolved strain-rate tensor, S, is obtained from the resolved velocity field and represents the local rate of deformation and rotation of the resolved flow structures.

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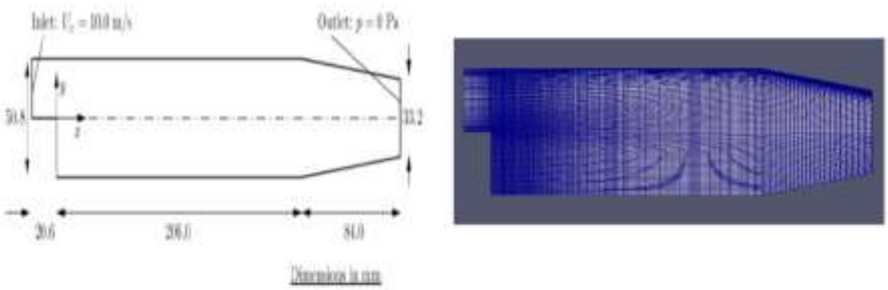
The LES turbulence modeling approach aims to resolve the larger turbulent structures through direct numerical simulation (DNS), while modeling the smaller, unresolved scales using the SGS model. This approach allows for a more accurate representation of the flow physics compared to Reynolds-Averaged Navier-Stokes (RANS) models.



(a) (b)

Figure 1: (a) Geometry & (b) Meshing of backward-facing step

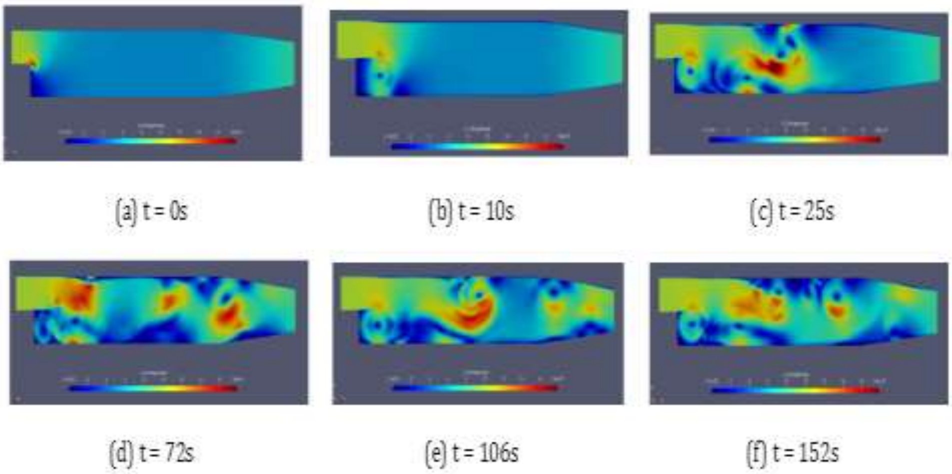


Figure 2: LES turbulence simulation of backward-facing step

2.2. Limitations of LES Turbulence Model

LES turbulence modeling in CFD presents several challenges that researchers have been working to address. Here are some of the key challenges associated with LES turbulence modeling:

1. Grid Resolution: LES requires fine grid resolution to capture the small-scale turbulent structures accurately. Resolving the full range of turbulent length scales can be computationally expensive, making it challenging to simulate complex engineering problems with high Reynolds numbers.

2. Subgrid-Scale Modeling: LES divides the flow into resolved and subgrid scales. Modeling the subgrid-scale (SGS) turbulence accurately is crucial for LES accuracy. Developing robust and accurate SGS models that can capture the complex interactions between resolved and unresolved scales is an ongoing challenge.

3. Near-Wall Modeling: Modeling near-wall regions accurately is critical in LES. The wall model should effectively capture the influence of wall boundaries on the resolved scales while accounting for the unresolved turbulent structures. Developing accurate and efficient wall models for LES is a challenging task.

4. Dynamic Adaptivity: LES simulations often require adaptive grid refinement to focus computational resources on regions of interest. Developing efficient and accurate adaptive mesh refinement techniques that can dynamically adjust the grid resolution based on flow characteristics is a significant challenge.

5. Sensitivity to Initial and Boundary Conditions: LES simulations are sensitive to the quality of initial and boundary conditions. Ensuring appropriate initialization and accurate boundary conditions that capture the inflow turbulence characteristics can impact the accuracy and stability of LES simulations.

Addressing these challenges requires collaborative efforts between researchers in the fields of CFD, turbulence modeling, and deep learning. By tackling these challenges, researchers aim to enhance the accuracy and efficiency of LES turbulence modeling, thereby improving the predictive capabilities of CFD simulations for a wide range of engineering applications.

3. METHODOLOGY

3.1. Dataset Generation

A complete dataset is developed by numerical simulations of the aforementioned governing equations on the mesh shown in Figure 1(b). The dataset consists of 33 columns & 25,012 rows. The developing fluid flow pattern in the computational domain is divided into 1000 timesteps to capture detailed dynamics. The Reynolds number (Re) at the inlet of the boundary is varied from 100 to 200 with an increment of 10. Hence, a comprehensive dataset comprising 11000 distinct pressure fields corresponding to each time step was created. The Coefficient of pressure at each timestep is non-dimensionalised by utilizing all-time maximum CoP at Re = 200. The data for varying the Reynolds number is shown in Figure 2 at different intervals of time.

3.2. Deep Learning Model

When developing the neural network architecture, the Navier–Stokes Equations inspired the selection of an FNO (Fourier Neural Operator). The network design incorporates four spectral convolution blocks and two fully connected layers, each comprising 128 neurons. The architecture is visually presented in Figure 3.

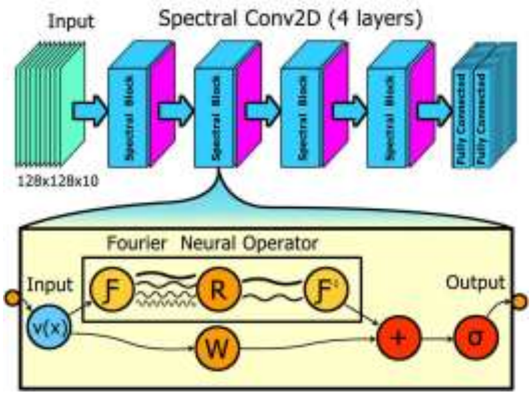


Figure 3: Deep Learning model based on FNO

In Figure 3 the F is the Fourier transform of a function f over the domain D, such that, $f : D \to \mathbb{R}^{d_v}$. The Fourier transform of the function f is then given by,

$$(Ff)_j(k) = \int_D f_j(x) e^{-2i\pi \langle x,k \rangle} dx \; ; \; j = 1, ..., d_v$$

(3.2.1)

& the inverse Fourier transform F^{-1} of equation 3.2.1 is given by,

$$(F^{-1}f)_j(x) = \int_D f_j(k) e^{2i\pi \langle x,k \rangle} dk \; ; \; j = 1, ..., d_v$$

(3.2.2)

The model accepts a sequence of 10 images as a single input in the form of a 3D array; every single input is with a shape of 128x128x10. We employ an image sequence generated from the CDF system, as explained in the dataset section. The original sequence is processed to create input blocks with ten images in each sequence at a particular time t.

Input_array[t] = ImageSequence[t : t+S]

(3.2.3)

where, represents a particular input time, and) represents an input sequence size for one block, which in our case, is set to 10.

A spectral convolution block consists of two streams. The FNO converts the input into the frequency domain and applies a low-pass filter to it, meaning that only the low-frequency content is considered in the multiplication between the Fourier transformed input and the systems Greens' function. Finally, the processed data is converted back to the existing domain. The weights used in the network to represent the spectral blocks are then combined with the weights that directly scale the input, as illustrated in Figure 3. An activation function is finally applied to obtain the block-wise output.

Now, when the domain D is discretized with $n \in \mathbb{N}$ points, uniformly with resolutions $s_1 \times s_2 \times .... \times s_d = n$, then the Fourier transform F can be replaced by the FFT (Fast Fourier Transform) $\hat{F}$

For $f \in \mathbb{R}^{n \times d_v}$, Fourier modes (k) will be $k = (k_1, \ldots, k_d) \in \mathbb{Z}_{s_1}, \ldots, \mathbb{Z}_{s_d}$, & $x = (x_1, \ldots, x_d) \in D$. The FFT $\hat{F}$ and its inverse $\hat{F}^{-1}$ is defined as ,

$$(\hat{F}f)_l(k) = \sum_{x_1=0}^{s_1-1} \ldots \sum_{x_d=0}^{s_d-1} f_l(x_1, \ldots, x_d) e^{-2i\pi \Sigma_{j=1}^{d} \frac{x_j k_j}{s_j}}$$

(3.2.4)

$$(\hat{F}^{-1}f)_l(x) = \sum_{k_1=0}^{s_1-1} \ldots \sum_{k_d=0}^{s_d-1} f_l(k_1, \ldots, k_d) e^{2i\pi \Sigma_{j=1}^{d} \frac{x_j k_j}{s_j}} \; ; \; l = 1, \ldots, d_v$$

(3.2.5)

3.3. Model Training, Validation & Evaluation

The flow of data and training methods utilized for the present study is shown in Figure 4. Data preprocessing is employed before furthering the data to the FNO model. This includes the resizing, centering, clipping, and aligning of the input image sequence. The preprocessed images are further processed to generate input sequenced blocks to match the model input shape of 128x128x10. The prepared data is split into training- and a test set sequence. The network is trained using a training loop, which employs loading the next batch, computes the loss function, updates optimiser and backpropagation derivatives for parameter updates. The model is saved at every best validation loss, and in case loss is not further improving, an early stop mechanism ends the training to avoid overfitting with the best weights in hand. Loss function for the training and test splits are shown in Figure 5.

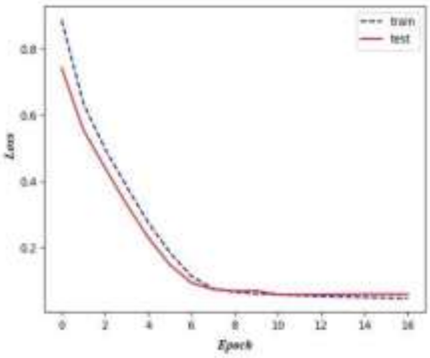


Figure 4: Model Implementation & Training Procedure **Figure 5:** Loss Function value for Train & Test Splits

4. RESULTS AND DISCUSSION

4.1 Performance Comparison with traditional LES Model

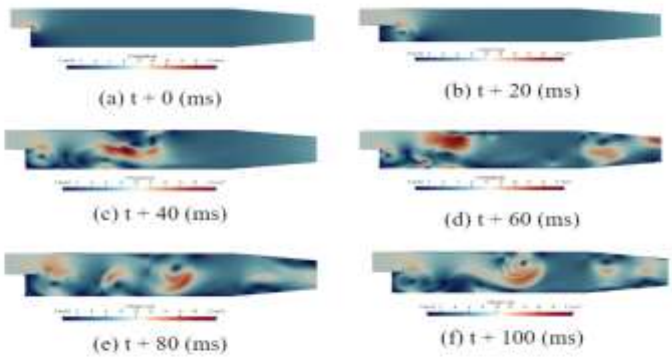


Figure 6: Enhanced LES Model using FNO in Deep Learning

The output sequence is generated based on the input development of the solution. CoP solutions at selected instances are displayed in Figure 6. While there are apparent visual differences between the Deep Learning Model (DLM) prediction and the traditional CFD simulation, they exhibit qualitative agreement. By comparing pixel-to-pixel binary images with a threshold pixel values we get that the pixel-to-pixel comparison for t+0ms is 1.303711%, for t+20ms is 1.227539%, for t+40ms is 1.218750%, for t+60ms is 1.290039%, for t+80ms is 1.361328% & for t+100ms it is 1.332439%, the solution prepared using the aforementioned deep learning model shows a high level of agreement with the solution generated through traditional CFD computations. Notably, the model successfully captures vortices generated in fluid past the backward-facing step. After providing the initial ten solutions at the beginning of the fluidstructure interaction (FSI), the subsequent ten solutions are purely predicted. The solution at the earliest instant, i.e., the 1st in the generated sequence, replaces the latest solution in the input sequence. This predict-and-replace process continues, and after 11 iterations, the entire input sequence is replaced with the predicted series of solutions. Starting from the 12th iteration until the 279th, all iterations are purely based on the predicted sequence of PDE solutions. The obtained results display divergent solutions at specific grid points. We believe that addressing this issue can be achieved by optimizing the network architecture, which is our future goal to attain state-of-the-art accuracy. Also the learned model proves useful for configuring the flow field, as demonstrated in Figure 6.

5. CONCLUSION

In conclusion, this research paper highlights the significant potential of leveraging deep learning techniques to enhance the Large Eddy Simulation (LES) turbulence model in Computational Fluid Dynamics (CFD). By addressing the limitations of traditional turbulence models, deep learning algorithms have been shown to improve the accuracy and efficiency of LES simulations. Through extensive training and validation on diverse datasets, the deep learning-based approach surpasses conventional LES models in predicting turbulent flows. The successful application of deep learning in turbulence modeling opens up new avenues for accurately simulating complex turbulent phenomena across various engineering and scientific fields. By harnessing the ability of neural networks to learn and capture intricate flow behaviors, the enhanced LES turbulence model offers an alternative to traditional models that struggle to capture the complexities of turbulence. Moreover, the use of deep learning has the potential to optimize computational efficiency, reducing the computational costs associated with LES simulations while maintaining high accuracy. While this research demonstrates promising results, it is important to acknowledge the challenges and limitations that come with implementing deep learning techniques in turbulence modeling. These include the requirement for substantial computational resources for training, the need for high-quality and diverse training data, and further investigation into the interpretability and generalizability of deep learning models across different flow conditions and geometries. In summary, this research paper contributes to advancing turbulence modeling in CFD by showcasing the efficacy of deep learning techniques in enhancing the LES turbulence model. The findings pave the way for future studies and encourage continued exploration of deep learning algorithms to improve simulation accuracy, deepen our understanding of turbulent flows, and facilitate practical applications in engineering and scientific disciplines.

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