Differentiable Turbulence: Closure as a PDE-constrained optimization

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Abstract

Deep learning is emerging as a powerful tool for enhancing sub-grid scale (SGS) turbulence models used in large eddy simulations (LES). By employing a differentiable turbulence solver and physics-inspired neural networks, we've developed highly accurate and adaptable SGS models for 2D turbulent flows. Our analysis reveals that incorporating small-scale non-local information is crucial for effective modeling, while large-scale features can refine the pointwise accuracy of the solution. We've demonstrated that the velocity gradient tensor can be directly mapped to SGS stress by decomposing inputs and outputs into isotropic, deviatoric, and anti-symmetric components. Our model excels in generalizing to various flow conditions, including different Reynolds numbers and forcing. We've compared our differentiable physics approach to offline, a-priori learning, finding that our hybrid solver-in-the-loop method offers the best balance of computational efficiency, accuracy, and generalization. Our findings provide practical guidelines for developing deep-learning-based SGS models that can effectively capture turbulence dynamics.

We propose a novel approach to data-driven turbulence modeling using differentiable computational fluid dynamics (CFD) solvers. By backpropagating a-posteriori errors to the turbulence model parameters, we can refine the model's accuracy. This 'differentiable turbulence' approach offers a distinct advantage over traditional machine learning methods like reinforcement learning, which often struggle with generalization to unseen flow conditions. While several previous studies have explored purely machine learning models for turbulence forecasting[Schiff et al., 2024, Brandstetter et al., 2022, Chakraborty et al., 2024], our approach leverages the underlying physics through a differentiable CFD solver. Figure 1 shows the architecture of the differentiable algorithm that we developed. Further details on the architecture is mentioned in Shankar et al. [2024].

We tried various ML models like Convolution Neural Networks(CNN), Fourier Neural Operators(FNO), Multi-Layer Perceptron(MLP) and their combinations. We trained the model on decaying turbulence at Reynold's Number(Re) 1000(DE) and tested to various other configurations like forced turbulence at Re 1000(G1), Re 30(G2), Re 10^5(G3) and Re 8000 with alternate forcing direction. Figure 2 shows that the model generalizes to various flow parameters along with improved performance compared to the Smagorinsky model for correlation with DNS. We found that non-locality and network architecture significantly influence performance and *a-posteriori* learning improves results

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1st Conference on Applied AI and Scientific Machine Learning (CASML 2024).

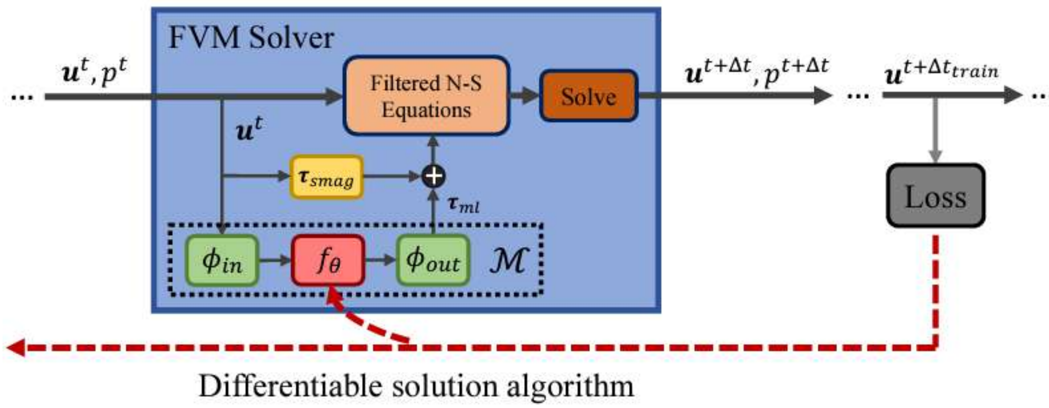

Figure 1: A diagram illustrating the deep learning-integrated solution algorithm. At each time step, the subgrid stress is calculated using a combination of the eddy-viscosity term (τ_{smag}) and a machine learning (ML) contribution (M). The ML contribution is generated by a neural network (f_θ) with trainable parameters, applied to transformed input (ϕ_{in}) and output (ϕ_{out}) data. The combined subgrid stress is then used in the LES equations, which are solved using standard numerical methods. The solution trajectory is compared to the ground truth DNS field, and a loss is calculated based on partial (i.e., subsampled) observations. Since the solution algorithm is differentiable, the loss can be backpropagated through all time steps and linear solves, allowing for updates to the neural network's trainable parameters.

compared to *a-priori* learning. Hybrid deep learning-solver algorithms offer potential for cheap and accurate CFD simulations due to their ability to incorporate physics. Future work will investigate the application of this approach to more complex wall-bounded flows.

Acknowledgements

This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 1745016 awarded to VS. The authors from CMU and Michigan acknowledge the support from the Technologies for Safe and Efficient Transportation University Transportation Center, and Mobility21, A United States Department of Transportation National University Transportation Center. This work was supported in part by Oracle Cloud credits and related resources provided by the Oracle for Research program. This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Advanced Scientific Computing Research (ASCR), under Contract No. DEAC02–06CH11357, at Argonne National Laboratory and Penn State University. We also acknowledge funding support from ASCR for DOE-FOA-2493 "Data-intensive scientific machine learning"

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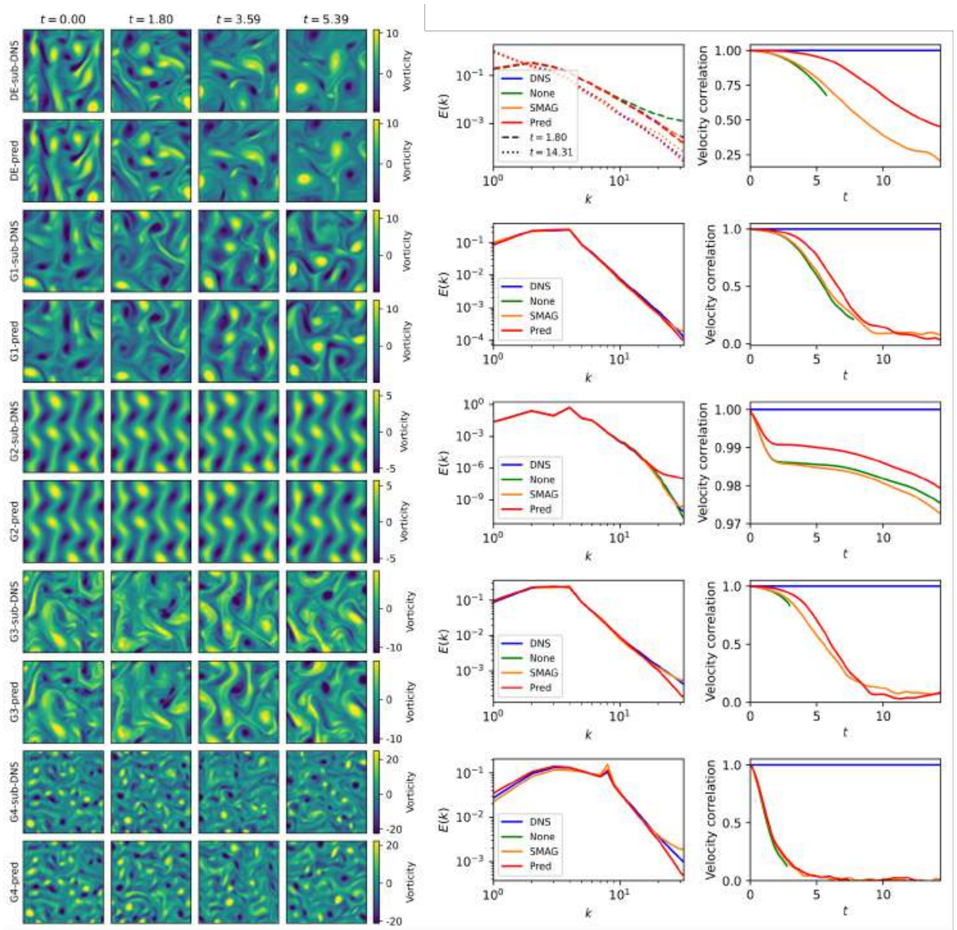

Figure 2: Summary of predictions from the CNN+FNO-MFS model. The left column displays an example predicted vorticity trajectory for each dataset compared with the true field. The right column shows the ensemble average energy spectra and velocity correlation over time for each dataset. Comparisons to baseline SMAG and no turbulence model are included. The CNN+FNO-MFS model improves over the baseline in both metrics for nearly every case. Only in the low Reynolds number dataset G2 does the model overpredict energy at the highest wavenumbers.