Aerodynamics and Fluid Mechanics
Engineering and Design
Technical University of Munich

Benchmarking ML models for Computational Fluid Dynamics

Semester Thesis/ Interdisciplinary Project (IDP) /Guided Research

The rapid advancement of machine learning (ML) has opened new frontiers in understanding and modeling complex fluid dynamics phenomena. Fluid dynamics, governed by the Navier-Stokes equations, underpins a wide range of applications, from weather forecasting and aerodynamics to energy systems and biomedicine. However, the inherent non-linearity and high-dimensional nature of these problems present challenges for traditional numerical solvers, particularly in scenarios that require large-scale simulations.

In this work, we explore the benchmarking of various state-of-the-art ML architectures like Transformers Herde et al. (2024), Diffusion models Kohl et al. (2023), Neural Operators (NOs) Li et al. (2020), Raonić et al. (2023), etc., on a curated set of fluid dynamics datasets as shown in Figure 1, emphasizing their predictive accuracy. By doing so, we aim to provide insight into the most suitable ML approaches for specific fluid dynamics scenarios and to promote a deeper understanding of their role in advancing this scientific domain. This benchmarking also establishes standardized evaluation metrics, fostering comparability between studies.

Milestones

- Review existing literature and repositories (Takamoto et al. (2022)) on selected state-of-the-art ML architectures.
- Develop a repository with the selected ML architectures.
- Investigation on different CFD datasets such as Kelvin Helmholtz instability, Double Shear Layer, Taylor Green Vortex etc.

Requirements

- Experience with Python (esp. Pytorch).
- Some knowledge of machine learning.
- Ability to work independently.

Optional

- Experience with computational fluid dynamics.
- Github workflows.

Contact

Harish Ramachandran harish.ramachandran@tum.de with the subject "Interested to contribute to the development of the benchmarking repository". Please also attach your CV, current grade report, and link to Github (if worked on any open-source projects).

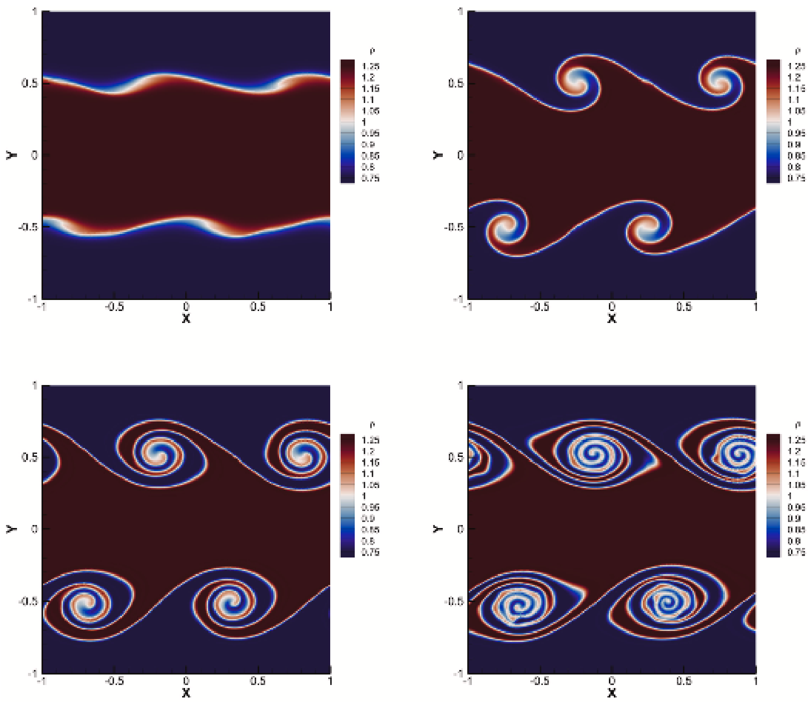

Fig. 6. Density at times $t = 2, 3, 4, 5$ for the Kelvin-Helmholtz instability test.

Figure 1: Density evolution of the Kelvin Helmholtz instability test

References

Herde, M., Raonić, B., Rohner, T., Käppeli, R., Molinaro, R., de Bézenac, E. & Mishra, S. (2024), ‘Poseidon: Efficient foundation models for pdes’.
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