Aerodynamics and Fluid Mechanics
Engineering and Design
Technical University of Munich

Invariant Features for Learning Equivariant Lagrangian Fluid Mechanics

Interdisciplinary Projects (IDP)

Lagrangian fluid mechanics is a way of solving the Navier-Stokes dynamics using a particle-based discretization of space. Machine Learning approaches to learning Lagrangian fluid mechanics are rather in their early stages, and benchmarking the performance of existing neural networks on such data is what brought the LagrangeBench project to life (Toshev et al., 2023a). We have already included the graph neural networks from Sanchez-Gonzalez et al. (2020); Brandstetter et al. (2021); Satorras et al. (2021); Schütt et al. (2021).

In this project, we want to add more machine learning models and benchmark them on the datasets included within LagrangeBench. We would start by implementing the recent SFBC model (Winchenbach and Thuerey, 2024) and drawing the connection between its Fourier features and the spherical harmonics bases typically used in equivariant machine learning (Toshev et al., 2023b). Then, the core of this project will be the reimplementation of the recent invariant feature-based model Ponita (Bekkers et al., 2023) in LagrangeBench. This model promises same expressive power and significant speedups compared to Clebsch-Gordan tensor product-based GNNs like SEGNN (Brandstetter et al., 2021). Related papers that would be helpful in the initial phase of the project and give more context are Sanchez-Gonzalez et al. (2020); Battaglia et al. (2016); Mrowca et al. (2018); Li and Farimani (2022); Toshev et al. (2023b).

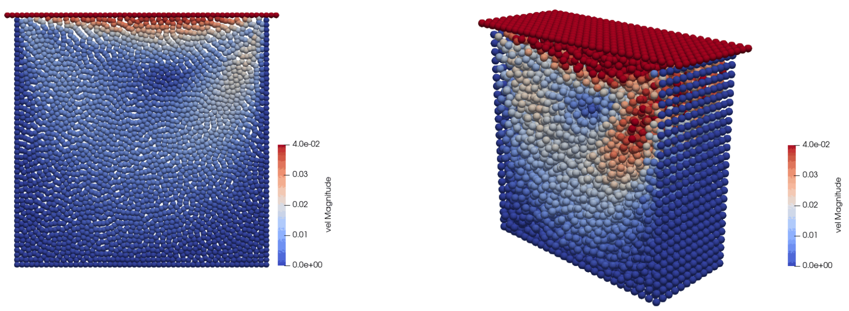

Figure 1: 2D and 3D lid-driven cavity simulation.

Milestones

- Reimplementing the two mentioned models in JAX and validating the code by reproducing one of the results from their respective reference papers.
- Integrating these models into LagrangeBench and benchmarking them.

Requirements

- Experience with Python, specifically JAX.
- Some knowledge of machine learning. GNNs or the specific models of interest are a plus.
- Ability to work independently.

Contact

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