Machine Learning algorithms in Computational Fluid Dynamics: Improving Reynolds-Averaged Navier-Stokes equations by ML closure models

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Short Abstract

Computational Fluid Dynamics (CFD) is a branch of fluid mechanics and numerical analysis that uses numerical methods and algorithms to analyze and solve problems involving fluid flows. CFD plays a crucial role in industry by providing detailed simulations of turbulent flows. Turbulence is a complex and chaotic state of fluid flows characterized by irregular fluctuations and mixing that significantly complicates their numerical simulation though the Navier-Stokes (NS) equations. A common approach to mitigate this issue is to solve the Reynolds-Averaged Navier-Stokes (RANS) equations that have as unknowns the averaged fields, thus avoiding the issue of solving for the fluctuations. However, RANS equations are not closed and require turbulence models to close the system of equations. Classic turbulence models based on heuristically-driven additional partial differential equations are usually inaccurate.

This thesis investigates the potential contributions of Machine Learning (ML) to the closure of RANS equations instead of using classic models. Recently, there has been a growing interest in exploiting ML algorithms trained on data from simple flows with Direct Numerical Simulation (DNS) results available to enhance the accuracy of traditional, heuristically-driven turbulence models. In this work, we introduce a novel model called the Vector Basis Neural Network (VBNN), followed by an improved version called turbulent viscosity-VBNN model, to close the RANS equations. The approach uses neural networks to infer the divergence of the Reynolds stress tensor, referred to as the Reynolds Force Vector (RFV). Numerical experiments demonstrate the effectiveness of this model. Furthermore, the thesis explores the natural coupling between ML-based turbulence models and Reduced Order Modeling (ROM). It also proposes an alternative to DNS to generate the simulations required to train ML algorithms using Delayed Detached Eddy Simulation (DDES), which allows for reliable and accurate simulations while maintaining reasonable computational costs. The thesis reports also results from two additional works: one that investigates the effect of the quality of the spatial discretization for the simulated flow around square cylinders, a paradigmatic case of interest in civil engineering, and one on the usage of neural networks in the framework of Virtual Element Method, a new emerging discretization technique.