Thesis Project: Machine Learning-Accelerated Solvers for Computational Fluid Dynamics Simulations

Topic

The computational work involved in computational fluid dynamics (CFD) simulations of viscous fluids, described by the stationary Navier–Stokes equations, can be extremely high since accurate solutions generally require fine mesh resolutions. In particular, depending on the Reynolds number of the flow, the Navier–Stokes equations may exhibit a highly nonlinear behavior, and the solution may be sought using nonlinear iteration methods, such as Newton's method, which amounts to solving a series of linear systems. For fine mesh resolutions, this often corresponds to the main portion of the computational work.

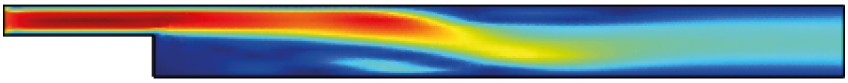

Figure 1: Backward-facing step flow.

So if the solution of large linear equation systems can be avoided or the number of solves can be reduced, this may significantly reduce the overall computational work and hence time. In previous work, the use of pseudo-time stepping methods [1] for accelerating the nonlinear convergence has been explored. Moreover, the definition of the local pseudo-time steps has been enhanced by the local use of neural networks (NNs), which often resulted in further acceleration; cf. [2]. Many questions, such as

- evidence-based selection of input features,
- further investigation of the locality of the NN models,
- investigation of feature importance, or
- adaptation of the involved network architectures

have remained open. This thesis project will follow-up on those open questions.

Milestones

1. Reproduction of the existing framework in an open-source numerical simulation framework such as OpenFoam or Fenics; see for instance Pseudo-Timestepping in OpenFOAM.
2. Work on improving the approach from [2] itself and better understanding its performance.
3. Evaluation for carefully chosen test cases, such as backward-facing step, lid-driven cavity, or Couette flow.

Required Skills

- **Research Skills:** Ability to conduct thorough literature reviews and gather relevant information
- **Analytical Skills:** Capability to analyze data and draw meaningful conclusions
- **Programming Skills:** Proficiency in Python and C++ (or a very strong will to self-teach)
- **Communication Skills:** Effective written and oral communication skills for documenting and presenting research findings
- **Demonstrated Experience:** Partial differential equations (PDEs), numerical simulations, machine learning
- **Teamwork:** Collaboration with peers and faculty members

Contact

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References

[1] C. Kelley and D. Keyes. Convergence analysis of pseudo-transient continuation. *SIAM Journal on Numerical Analysis*, 35, 08 1996. doi: 10.1137/S0036142996304796.

[2] A. Zandbergen, T. van Noorden, and A. Heinlein. Improving pseudo-time stepping convergence for cfd simulations with neural networks, 2023.