Predicting the Optimal Solver Settings with Machine Learning in COMSOL CFD Module

Improving the COMSOL solver choice for CFD by predicting the optimal solver parameters with the use of Machine Learning

Performing computational fluid dynamics (CFD) simulations and analysing fluid flows can be very complex, especially for transonic or turbulent flows. Choosing the right solver settings can therefore be very important for obtaining a (precise) solution in low computing time. This is however often not straightforward. Simulation software packages that perform finite element analyses (FEA) generally provide default solver settings to improve the usability, in particular, for non-expert users. However, these default solver settings do not always result in the fastest convergence of the linear/nonlinear solvers, and moreover, they can even result in divergence for difficult problems. In many cases, by fine-tuning the parameters, convergence can be achieved or accelerated significantly. A machine learning model that can predict a good set of solver settings can offer a solution to this problem.

In this thesis project, we will investigate the prediction of solver parameters using a machine learning model, such that a fast converged solution can be achieved. In particular, a neural network will be trained to predict the optimal solver parameters of different laminar flow CFD models in COMSOL [1]. As the training data we will use a data set containing information from the convergence history of simulations. This offline phase is computationally expensive; however, the prediction of the solver parameters will then be fast. Different configurations of laminar flow problems will be considered in order to enable generalization of the neural network to a large range of laminar flow models.

We will investigate using both global and local information of different laminar flow CFD models in COMSOL and train a neural network to predict the optimal parameters. Global information could be geometry information or initial conditions, and local information could be, for instance, velocities, pressure, residuals, or the Reynolds number for each individual finite element. We would prefer using local data because we expect better generalization properties of the resulting neural network model, and possibly one CFD simulation already contains enough data to train the neural network; cf. [2,3].

Since this is a new research topic, there are a lot of open questions about which input to use, how to design the network architecture, and how to determine and tune the solver parameters from the output of the neural network.

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Start of the project: December 2021
This work is done in collaboration with Tycho van Noorden in the CFD development department of COMSOL

[1] COMSOL Multiphysics Software - Understand, Predict, and Optimize. https://www.comsol.com/comsol-multiphysics

[2] Nils Margenberg et al. “A neural network multigrid solver for the Navier-Stokes equations”. In: Journal of Computational Physics (2022), p. 110983. ISSN: 0021-9991. http://dx.doi.org/10.1016/j.jcp.2022.110983

[3] Deep Ray and Jan S. Hesthaven. “Detecting troubled-cells on two-dimensional unstructured grids using a neural network”. In: Journal of Computational Physics 397 (2019), p. 108845. ISSN: 0021-9991. https://www.sciencedirect.com/science/article/pii/S0021999119305297