Delft University of Technology

Project: Improving Nonlinear Solver Convergence Using Machine Learning

Supervisor(s):
Alexander Heinlein (Numerical Analysis, EEMCS)
Tycho van Noorden (COMSOL)

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1 Project Description

The simulation of fluid flows has applications in a broad range of research and engineering problems in many areas of study and industries. In many instances, a steady state solution is required of a model involving the Navier–Stokes equations. After discretizing these equations, a system of equations is obtained. Since these equations are inherently nonlinear, an iterative procedure, such as the Newton–Raphson method, is needed for the numerical solution of the equations.

The convergence of these iterative procedures depends strongly on a good initial guess of the solution. For instance, the Newton–Raphson method converges quadratically in the vicinity of the solution, however, it may converge slowly or even diverge far away from the solution. Unfortunately, a good initial iterate is not always easy to guess or to construct, especially for geometrically more complex models. To overcome convergence issues for the nonlinear solvers, globalization techniques (see, e.g., [2]) can be employed, for instance, pseudo-time stepping. This technique tries to mimic the dynamic time-stepping of an initial condition towards a steady state, but instead of choosing the time step size based on accuracy criteria, it tries to choose the time step size in order to obtain robust, yet fast convergence to the steady state solution; see, e.g., [1]. In addition, since the intermediate solutions are not of interest, the pseudo-time stepping technique has the freedom to choose different time steps for each cell or mesh element if that speeds up the convergence.

The work in the thesis [3] shows that a neural network can be trained to use local data from the triangular finite element mesh to predict local time step sizes, via so-called local CFL (Courant–Friedrichs–Lewy) numbers, that lead to faster and more robust convergence than conventional pseudo-time stepping algorithms for 2D, incompressible laminar flow simulations. In addition, the fact that the neural network uses local data makes it easy to apply the network predictions to any other flow simulation that uses a triangular mesh, and in [3], it is shown that the approach generalizes well for a range of different 2D flow simulations.

The aim of this project is to extend the work in [3], and since the research topic is rather new, this can be done in quite a number of different directions:

- Extend the work in [3] by applying the method to other flow simulations, e.g.,
  - 3D flow,
  - turbulent flow,
  - compressible flow,
  - etc.
- Extend the work in [3] by investigating the method itself:
  - Investigate the influence of the type of neural network used (e.g., recurrent networks)
  - Investigate what the best input data is for the network, by, e.g., scaling or simplifying the local mesh data
  - Directly predict local time step sizes instead of local CFL numbers
  - Investigate different loss functions to train the network
  - etc.

Prerequisites

Sufficient knowledge of fluid mechanics, finite elements and machine learning, as well as good programming skills (Matlab) are required. In addition, experience with COMSOL Multiphysics is recommended.

Contact

If you are interested in this project and/or have further questions, please contact Alexander Heinlein, a.heinlein@tudelft.nl, and/or Tycho van Noorden, Tycho.vanNoorden@comsol.com.

References

[1] C. T. Kelley and D. E. Keyes. Convergence analysis of pseudo-transient continuation. *SIAM Journal on Numerical Analysis*, 35(2):508–523, 1998.

[2] R. P. Pawlowski, J. N. Shadid, J. P. Simonis, and H. F. Walker. Globalization techniques for Newton–Krylov methods and applications to the fully coupled solution of the Navier–Skes equations. *SIAM review*, 48(4): 700–721, 2006.

[3] A. Zandbergen. Predicting the optimal CFL number for pseudo time-stepping with machine learning in the COMSOL CFD module. Master's thesis, Delft University of Technology, 9 2022.