MSc. Thesis Proposal

Title: Poisson Equation Linear Solvers based on Machine Learning

Supervisors

Tiago Gomes (MSc): CFD Development & Application at blueOASIS
Guilherme Vaz (PhD): R&D manager at blueOASIS
Professor at Instituto Superior Técnico

Introduction

Motivation

CFD is an important engineering tool, which despite having benefited from advances in available computational power, can still be very time consuming in many situations. One bottleneck lies in the solution of the pressure field, a Poisson equation, to respect continuity in incompressible flows. The resulting linearized system of equations is iteratively solved using traditional methods (e.g., Jacobi, CG, GMRES, etc.), yet this step can represent up to 90% of the overall computational time. This is where Machine Learning has the disruptive potential of significantly reduce the solution time, either by providing a better guess of the linear system's solution to the traditional solvers or substituting them altogether.

Existing work

Tompson et al. [1] used a data-driven approach with Convolutional Neural Networks (CNNs) to accelerate the pressure projection step in Eulerian (inviscid) fluids for computer graphics. It included several data augmentation techniques to increase the accuracy and stability of the ML solver. Moreover, the divergence of the resulting velocity field, a measure of the quality of the pressure field predicted to respect continuity, was selected for the loss function. This unsupervised learning architecture is advantageous since it does not rely on a ground-truth calculated by classical solvers and infuses essential physics into the ML algorithm (see importance of PINNs in the seminal work by Karniadakis et al. [2]). Illarramendi et al. ([3], [4]) continued this work and further refined and adapted the methodology towards engineering CFD solvers. By merging the ML solver with a classical one, a hybrid tool was created that enables user-defined accuracy to be reached, with overall good performance even in previously unseen data.

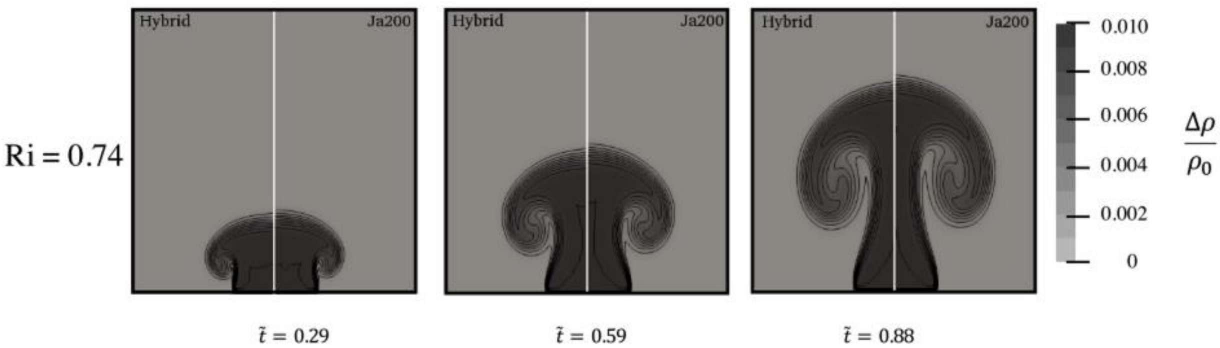

Figure 1: Hybrid solver vs. classical Jacobi solver [3].

Objectives

The objective of this thesis is:

- To analyze existent open-source ML-based linear solvers that can be used for Poisson equations;
- To investigate innovative approaches to the problem, e.g. working directly with the matrix values of the linear system as pixels in an image;
- To couple a ML-based solver, based on the results of the previous two points, with the CFD solver ReFRESCO (www.refresco.org);
- Run several benchmark test cases to evaluate the performance of the ML solver against traditional ones.

The expected tasks are:

- Literature review on the existing methodologies;
- Investigation and experimentation with available open-source solutions;
- Research and development of a new approach to the issue (see above);
- Coupling of one ML solver with ReFRESCO;
- Generation of test cases, including training data, to assess its performance.

Requisites

Applicants must have:

- General knowledge on Artificial Intelligence.
- General knowledge on Fluid Dynamics and CFD.
- Affinity with data processing.
- Coding experience with Python or similar.

Good to have:

- Linux experience.
- LaTeX experience.
- Git experience.
- Coding experience with FORTRAN90 or newer.

Location

blueOASIS (www.blueoasis.pt) Edifício D. Pedro, Quinta da Fonte, R. Malhões, 2770-071 Lisboa or Ericeira Business Factory, R. Prudêncio Franco da Trinitade 4, 2655-344 Ericeira.
The student must be present at the office **at least 4 days per week**. This is mandatory to pursue a thesis with blueOASIS.

Companies Involved

blueOASIS is a young team with more than 65 years of combined knowledge and experience on Aerospace, Mechanical, Naval and Maritime engineering. The multicultural and multidisciplinary team is committed to make our oceans safer and greener, using state of the art numerical and data science tools. BlueOASIS focuses on renewable energies, ocean cleaning, decarbonization, sustainable offshore structures and green ships optimization.

Bibliography

[1] J. Tompson, K. Schlachter, P. Sprechmann, and K. Perlin, "Accelerating eulerian fluid simulation with convolutional networks," *34th International Conference on Machine Learning, ICML 2017*, vol. 7, pp. 5258–5267, 2017.

[2] G. E. Karniadakis, I. G. Kevrekidis, L. Lu, P. Perdikaris, S. Wang, and L. Yang, "Physics-informed machine learning," *Nature Reviews Physics*, vol. 3, no. 6, pp. 422–440, Jun. 2021, doi: 10.1038/s42254-021-00314-5.

[3] E. A. Illarramendi, M. Bauerheim, and B. Cuenot, "Performance and accuracy assessments of an incompressible fluid solver coupled with a deep Convolutional Neural Network," pp. 1–31, 2021, [Online]. Available: http://arxiv.org/abs/2109.09363

[4] E. A. Illarramendi, M. Bauerheim, and B. Cuenot, "Performance and accuracy assessments of an incompressible fluid solver coupled with a deep convolutional neural network," *Data-Centric Engineering*, vol. 3, no. 8, pp. 1–31, 2022, doi: 10.1017/dce.2022.2.