POLITECNICO
MILANO 1863

SCUOLA DI INGEGNERIA INDUSTRIALE
E DELL'INFORMAZIONE

Project Report

Title

Advanced Programming for Scientific Computing

Authors: Andrea Bonifacio, Sara Gazzoni

Advisors: Stefano Pagani

Co-advisor: Mattia Corti

Academic year: 2022-2023

---

1. Introduction

Full 3D blood flow models are important in the study of cardiovascular system since they allow to extract detailed quantities of interest but their actual implementation is limited due to their high computational cost. For this reason, reduced order models are widely used in this fields because of their efficiency. An example is presented in [2], where a one-dimensional reduceced order model is implemented to simulate the blood flow in the aorta using a graph neural network trained on three-dimensional simulations. In this work, we propose a different application, where the graph neural network is used to approximate the solution of different problems. In particular, we consider the heat equation as test case, but the goal of the project is to show the potential extension of this approach to solve more difficult problems with complex geometries, such as the simulations of proteins spreading in the neural system, which are at the basis of neurodegenerative diseases [1]. The main part of this project is the implementation of a library for data generation used to train the graph neural network and the adaptation of the code [di Luca non so come citarlo] to make it suitable for our specific test case. In the following sections, we first present the problem formulation and a detailed description of the code developed, then we show the results obtained and a discussion of the possible further developments and extensions.

2. Problem overview

We consider a general time-dependent variational problem of the form:

$$Lu = f$$

with L a linear operator, f a source term and u the solution. Given a specific geometry Ω and using the finite element method implemented in Fenics, we can solve this problem and obtain the solution u^n at each time step n. From this, we can generate a graph that decribes the geometry of the problem and the solution, storing some values of interest as features of the nodes and the edges. Solving the problem for different geometries and different values of the parameters (e.g. the diffusivity constant) we can generate a dataset that will be used to train the graph neural network. As in [2], the GNN is applied iteratively: at each time step it takes as input the system state Θ^n, which is the set of all the nodes and edges features at that time step, and it predicts an update for the state variables. The prediction is combined with the previous time step to estimate Θ^{n+1}.

2.1. Test case: heat equation

In this work, we consider the heat equation as test case. The mathematical formulation of the problem is the following:

$$\begin{cases} \frac{\partial u}{\partial t} = k\Delta u \quad \text{in } \Omega \subset \mathbb{R}^2, \\ \frac{\partial u}{\partial n} = h \quad \text{on } \partial\Omega_{inlet}, \\ \frac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega_{outlet} \cup \partial\Omega_{walls}. \end{cases} \tag{1}$$

where u is the temperature, k is the diffusivity constant, h is the Neumann condition at the inlet boundary. As domain Ω we consider different geometries such as the one shown in Figure **??**:

We generated 20 different mesh using gmsh. Then we solved the problem in Fenics using Discontinuous Galerkin method and implicit Euler for time discretization, imposing as Neumann condition at inlet $h = 2e^{-(t-2.5)^2}$.

3. Code

4. Results

5. Further work

References

[1] Mattia Corti, Francesca Bonizzoni, Luca Dede', Alfio M. Quarteroni, and Paola F. Antonietti. Discontinuous galerkin methods for fisher-kolmogorov equation with application to alpha-synuclein spreading in parkinson's disease. *Computer Methods in Applied Mechanics and Engineering*, 2023.

[2] Luca Pegolotti, Martin R. Pfaller, Natalia L. Rubio, Ke Ding, Rita Brugarolas Brufau, Eric Darve, and Alison L. Marsden. Learning reduced-order models for cardiovascular simulations with graph neural networks. *Computers in Biology and Medicine*, 2023.