CEMRACS 2023 mini-project proposal

Title: Fourier Neural Operators for Incompressible Two-Phase Flow simulation
Contact: Thibault Faney
Institution or company: IFP Energies Nouvelles
Email: Thibault.faney@ifpen.fr

1. Context

Define the scientific and technological context with a brief state of the art.

Data-driven algorithms for the resolution of Partial Differential Equations (PDEs) have recently seen an important resurgence, from finite dimensional operators learning solutions on a fixed discretized mesh using Convolutional Neural Networks (CNN) [1] to Physics Informed Neural Networks (PINN) learning to directly minimize the residual of a given PDE [2]. Unfortunately, these approaches suffer from a lack of generalization capabilities with respect to PDE coefficients, boundary and initial conditions, mesh discretization and domain geometry.

Neural Operators (NO) have alleviated some of these concerns by learning directly mesh-free, infinitely dimensional operators [3], however the computational cost of evaluating integral operators remained prohibitive. More recently, Fourier Neural Operators (FNO) have alleviated this issue by learning directly in Fourier space, thus speeding up both training and inference time [4]. Since then, several methods have improved upon this work with impressive results on a large variety of applications [5]–[7].

2. Description and objectives

Describe the proposed mini-project and state the foreseen results, if possible with quantitative metrics.

This mini project aims at evaluating recent advances in FNO in the context of Darcy flow PDEs that model applications such as CO2 sequestration or geothermal energy. A simple but useful Darcy flow model is the incompressible two-phase flow, modeled by a system of PDEs:

$$\left.\begin{aligned} &\phi\frac{\partial S_\alpha}{\partial t} + div(v_\alpha) = q_\alpha \\ &v_\alpha = -K\frac{k_r(S_\alpha)}{\mu_\alpha}\nabla P \end{aligned}\right. \quad \text{for } \alpha = w, g$$

where the unknowns are the pressure P and the saturation of the gas and aqueous phases S_g and S_w, with the closure equation $S_g + S_w = 1$. φ and K are the porosity and the permeability fields, k_r is a non-linear relative permeability law depending on the saturation, μ_g and μ_w are the gas and water viscosities, and q_g and q_w are the gas and water injection source terms (e.g. corresponding to well injection events).

We are especially interested in the ability of FNO to generalize to various permeability fields K and/or to various locations of gas injection source terms q_g. Note that the permeability field is a function defined on the whole spatial domain, and that the source terms are functions defined on a variable but specific location in the domain. This makes this project potentially more difficult than some traditional work addressing generalization for scalar parameters.

The metrics evaluating the results are the accuracy of the solution (with respect to a reference solution computed using a fine grid simulation), and the inference time for evaluation of the FNO on test data.

3. Proposed methodology

Describe the proposed methodology for the realization of the mini-project.

Starting from a provided python solver for the incompressible two-phase flow equations on a 2D geometry, the first part of the project consists in defining a design of experiments with various permeability fields and source term locations, performing the corresponding simulations, and aggregate the resulting data to form a training database. As a simplifying assumption, permeability fields will be drawn from a lognormal distribution.

The second part consists in training the FNO and evaluating the performance on previously unseen data. Depending on the success with the initial FNO algorithm, a modified version incorporating the residual loss of the equation [5] can be implemented, allowing to incorporate more physics induced biases in the training.

4. Software requirements

List the required software for implementing the mini-project.

The mini-project will be performed entirely using the python programming language. The python solver for the PDE system is provided, and the python code for the FNO implementation is available at https://github.com/neural-operator/fourier_neural_operator .

5. References

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