Multi-scale simulation with physics-informed neural networks

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Background

Scientific research relies on our ability to **simulate** scientific phenomena. From understanding how biological systems interact to modelling the evolution of the universe, simulations allow us to predict properties, test hypotheses, and explore scenarios that might be difficult to investigate experimentally. Many of the physical systems we are interested in studying today exhibit strongly **multi-scale** phenomena. These systems are characterised by their complex interactions across multiple spatial and temporal scales, for example, the interaction of clouds with atmospheric circulation in global climate models, or the formation of hierarchical dark matter structures.

Accurately carrying out multi-scale simulation poses a significant challenge, as it requires sophisticated models that can correctly capture these interactions. Moreover, the **computational cost** of traditional numerical simulation (such as finite difference and finite element modelling) can be immense, requiring the use of supercomputers for each simulation.

In recent years, the field of **scientific machine learning** has offered new ways of overcoming these challenges [1]. For example, **physics-informed neural networks** (PINNs) [2,3] are a way to carry out simulations using neural networks. In contrast to traditional numerical methods, they do not require complex simulation meshes and they can easily incorporate observational data to learn about interactions. However, using PINNs out-of-the-box comes with significant challenges; they can be **computationally expensive** to train and can struggle to model multi-scale interactions.

Our recent work [4,5] showed that PINNs can carry out multi-scale simulation effectively by combining them with **domain decomposition** and **multilevel modelling**. Domain decomposition allows the global simulation problem to be decomposed into smaller, easier-to-solve problems, whilst multilevel modelling provides better communication between multi-scale interactions.

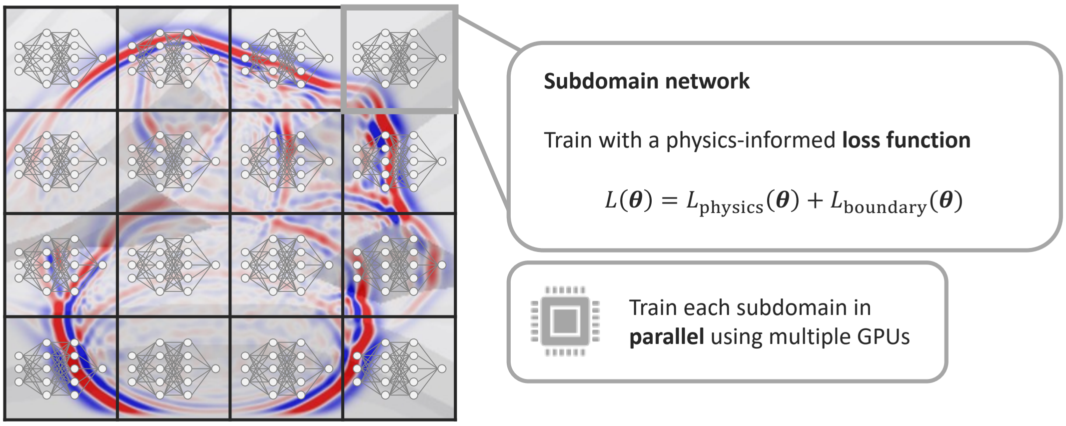

Figure 1: Multi-scale simulation with physics-informed neural networks. In our recent work, we propose a method for multi-scale simulation which combines physics-informed neural networks with **domain decomposition** and **multilevel modelling**. The simulation works by dividing the modelling domain into many subdomains, placing separate neural networks in each subdomain, and training the networks in parallel using a physics-informed loss function. Example shown is using our method to simulate seismic waves in an earthquake.

Project

The goal of this project is to investigate whether PINNs can carry out large, multi-scale simulation efficiently and accurately. We will extend our existing method so that it trains across multiple GPUs, allowing arbitrary hardware scaling. We will also investigate algorithmic improvements for improving efficiency and accuracy, such as adaptively learning domain decompositions.

A major goal is to be able to carry out realistic multi-scale simulations, such as turbulent fluid dynamic simulations with high Reynolds numbers (for example, modelling the Earth's climate), and inhomogeneous wave simulations (for example, modelling regional earthquakes). Another goal is to use the PINN to learn multi-scale interactions from observational data. Key research questions are: how do PINNs compare to traditional numerical methods when carrying out multi-scale simulation? What are effective ways of modelling multi-scale behaviour with PINNs? How does accuracy and convergence scale with problem size?

Please see the official GitHub repository for our existing code:
https://github.com/benmoseley/FBPINNs

Impact

Efficient and accurate multi-scale simulation methods will have a transformative impact on science. They will allow us to better understand the impact of complex interactions in physical systems, and lead to more accurate predictions and understanding in fields such as climate modelling, materials science, and biological systems. There are many impactful simulation tasks across the Department of Earth Science and Engineering which could be studied.

Supervision

Dr. **Ben Moseley** is a Lecturer in AI (Schmidt AI in Science Fellow) at the Department of Earth Science and Engineering and a fellow at the Imperial I-X Centre. He heads the scalable scientific machine learning lab and is an expert in scientific machine learning, physics-informed neural networks, neural differential equations, hybrid modelling, learned inverse algorithms, high-performance computing, geophysics, and planetary data science.

We are open to identifying a further co-supervisor or project advisor as necessary. We actively encourage collaboration with industry and other research groups.

Research group

The student will be part of the **scalable scientific machine learning lab** headed by Dr. Ben Moseley. The lab accelerates scientific research by designing scientific machine learning algorithms and applying them to impactful problems across Earth science, space science, and other domains.

We value **interdisciplinarity** – we train our members across machine learning, applied mathematics, high-performance computing, and in domain-specific areas including geophysics, climate science, and planetary science. We **collaborate** with other groups at the Department of Earth Science and Engineering, I-X (Imperial's AI initiative), other Imperial departments, and with external universities and industry partners. Lab members are encouraged to present and publish at high-impact conferences and journals.

Student profile

We are looking for someone who is motivated to complete a PhD in scientific machine learning, high performance computing, and multi-scale modelling across scientific domains. Given the interdisciplinary nature of this project and group, we do not expect candidates with deep experience in all areas; instead, we are looking for someone who has a strong foundation, a willingness to work across disciplines, a passion for continuous learning, and the ability to approach complex problems with creativity and curiosity.

Essential qualifications / experience:

- Good Master's degree in a relevant field, e.g. mathematics, physics, computer science, engineering, or Earth science. Motivated candidates with an excellent bachelor's degree and a relevant research portfolio are encouraged to apply
- Completed courses in machine learning and/or applied mathematics / numerical modelling

- Coding proficiency in e.g. Python/ C++/ Julia/ Fortran

Desirable qualifications / experience:

- Understanding of numerical modelling (finite difference, finite element, spectral methods, multilevel methods, etc)
- Understanding of scientific machine learning, in particular physics-informed neural networks
- Familiarity with different deep learning architectures
- Proficiency with Python machine learning frameworks (PyTorch, JAX (with Equinox))
- Experience in scientific, HPC, GPU, and/or parallel computing
- Relevant publications and/or industry experience are a plus

Funding

This project is not currently funded through a research grant and is eligible for College and/or Departmental scholarship funding. For more details on scholarship funding and deadlines see here: https://www.imperial.ac.uk/earth-science/prosp-students/phd-opportunities/funding/

Apply

If you are interested, please start by sending us a CV and detailed description (~200-400 words) of your relevant experience and specific research interests.

For more details on the Imperial PhD application process see here: https://www.imperial.ac.uk/earth-science/prosp-students/phd-opportunities/

Contact

Ben Moseley will be joining Imperial in November 2024. Before this date, please visit his personal website for contact details: https://benmoseley.blog/

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