# Multi-scale simulation with physics-informed neural networks

Supervisor: Ben Moseley

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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]. **Physics-informed neural networks** (PINNs) [2,3] are a popular 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 often struggle with issues such as spectral bias.

Our recent work [4,5,6] 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.

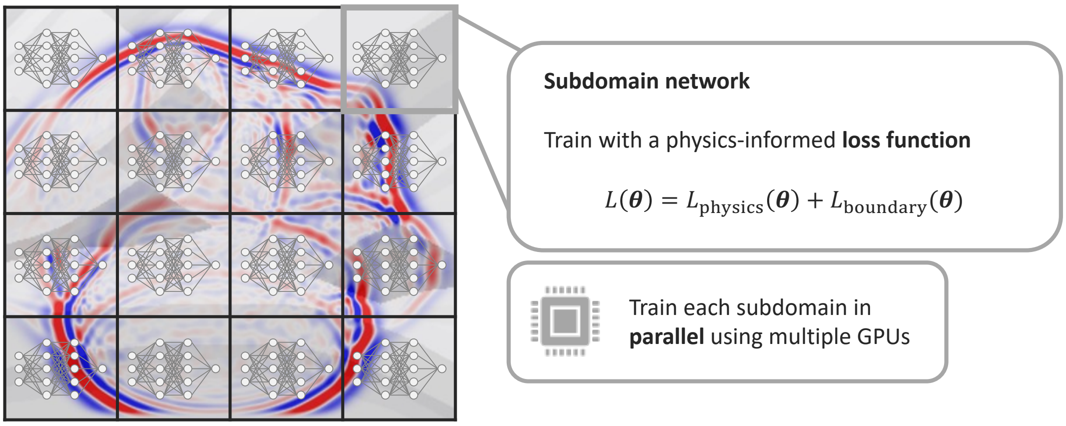


Figure 1: Multi-scale simulation with physics-informed neural networks. The simulation works by dividing the modelling domain into many subdomains, placing separate neural networks in each subdomain, and training the networks in parallel using a physics-informed loss function. Example shown is using our method to simulate seismic waves in an earthquake.

## Project

The goal of this project is to **design PINNs which can carry out large, multi-scale simulations efficiently and accurately**. We will extend our existing methods so that they can train across multiple GPUs, allowing arbitrary hardware scaling. We will also investigate algorithmic improvements for improving efficiency and accuracy, such as adaptively learning domain decompositions and using random feature methods and linear solvers (see [6]) to accelerate training.

A major goal is to carry out real-world multi-scale simulations, such as turbulent fluid simulations with high Reynolds numbers (for example, modelling the Earth's climate), and inhomogeneous wave simulations (for example, modelling regional earthquakes), working with domain-specialist teams across Imperial.

**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?

For more details: please see our project page and GitHub repository.

## 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.

## Supervisory team

Dr. **Ben Moseley** is an Assistant Professor 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 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 science. See our lab website for more information.

We are a highly **cross-disciplinarity** team – 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. This is an interdisciplinary project, and we do not expect candidates to arrive with expertise in all areas; instead, we are looking for someone with a strong technical foundation, enthusiasm for interdisciplinary research, and an ability to approach complex problems with creativity and curiosity.

Essential qualifications / experience:

- Good Master's degree in a relevant field (e.g. applied mathematics, physics, computer science, engineering, or related areas). 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
- Coding proficiency in e.g. Python/ C++/ Julia/ Fortran

Desirable qualifications / experience:

- Experience in numerical modelling (finite difference, finite element, spectral 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.

## Apply

If you are interested, please start by sending us:

- CV (including education, and any research experience).
- Brief motivation letter (200 – 400 words) where you should highlight how your experience enables you to pursue the project (can be in the email body).
- Any additional materials that support your application (optional).

For more details on our lab's PhD application process see here.
For more details on the Imperial PhD application process see here.

## Contact

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### References

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