Large scale AI modelling for Environmental Flows
Dr Claire Heaney, Prof. Christopher Pain

Background
Due to the rapidly increasing availability of data (sensors, the internet of things), much research effort is being focused on the improvement of computational models and their forecasts by combining them with data and with machine learning techniques, adept at handling data. For real-world problems, computational models are capable of providing high resolution simulations although this can take weeks of simulation time on a cluster. Reduced-order modelling (ROM) has received much interest over the last decade, and has the potential to revolutionise many-query problems (such as data assimilation and uncertainty quantification), which were previously constrained by the computational intractability of needing to solve a high-fidelity problem many times. Instead of expanding the solution in terms of simple, piecewise, low order polynomials (as done in the Finite Element method for example), ROM seeks global basis functions which contain much information about the behaviour of the system. As a result, many fewer of these global basis functions are required, and so the dimension of the problem reduces to something that is very fast to solve (for example from millions of degrees of freedom to hundreds). Non-intrusive ROM (NIROM) (or data-driven ROM) has been developed to tackle problems in which the high-fidelity model is based on legacy code or requires the solution of complex, coupled problems. Instead of relying on a projection to the low-dimensional space defined by the basis functions, NIROM performs an interpolation, which is nowadays often done by neural networks (NN). One challenge for these models is that, when predicting, the solutions can stray beyond the limits of the knowledge of the NN (based on the training data), leading to unrealistic results and divergence.

Adversarial networks, such as Generative Adversarial Networks (GANs) and Adversarial Autoencoders (AAE), are able to generate more realistic-looking images than standard feed-forward networks. When applied to computational physics scenarios, the aim is that these networks will produce a solution that does not diverge and predicts realistic behaviour. Physics-Informed Machine Learning is another technique that can constrain the network to produce physically realistic behaviour by introducing some of the physics of the underlying problem into the network. Domain decomposition (DD) methods have been applied to high-fidelity models to enable large models to run on clusters in parallel. They can also be applied to ROMs for similar reasons. Models are formed locally using DD-NIROMs and these are linked together to form large scale AI models.

Project
This project will aim to make significant progress by improving NIROM methods by incorporating state-of-the-art techniques from the field of machine learning and hence, contributing to the fast-growing field of digital twins. GANs and AAEs will be extended so that they predict in time, assimilate data (which comes naturally through their backwards propagation), and uncertainties will be derived from their solutions. Loss functions of the neural networks will be enriched by residual terms from continuity, momentum or energy equations, in an attempt to constrain the neural networks to physically realistic trajectories. These technologies will be set in a domain decomposition framework to tackle large-scale problems. The ‘digital twins’ that are produced within this project will be tested on a challenging problem from the field of environmental flows, such as flows in urban environments or geothermal flows.

Candidate
The candidate should have a strong mathematical background, a good degree in an appropriate subject (eg. mathematics, physics, computer science, engineering or earth sciences), and a strong interest in computational modelling and code development. The student will be joining one of the largest research groups at Imperial, namely the Applied Modelling and Computation Group (AMCG), with experience in computational fluid dynamics, urban flows, flooding, multiphase flows, porous media, geothermal engineering, reservoir modelling. The candidate will have the opportunity to develop their career and profile by presenting at conferences and publishing in high impact journals.

Funding details / Application
Unfortunately, there is no funding associated with this PhD topic. Please see the following pages for advice on applying for scholarships
https://www.imperial.ac.uk/study/pg/fees-and-funding/scholarships/
https://www.imperial.ac.uk/earth-science/prosp-students/phd-opportunities/funding/

For more information about the project please contact Claire Heaney (c.heaney@imperial.ac.uk) or Christopher Pain (c.pain@imperial.ac.uk).

For details on how to apply please consult
https://www.imperial.ac.uk/earth-science/prosp-students/phd-opportunities/apply/.