School of Mathematical Sciences
PhD studentship in Mathematical Sciences

Model reduction and homogenisation for filtration and adsorption

Supervised by Dr Matteo Icardi (Mathematics) and Dr. Bagus Muljadi (Engineering)

This project will be based at the University of Nottingham in the School of Mathematical Sciences in the group of Industrial and Applied Mathematics, and in collaboration with the GeoEnergy Research Centre.

Porous media are ubiquitous in natural and engineered transport processes. When colloids or diffusive particles flows through their complex geometrical structure, non-trivial interactions arise between the advection, diffusion, particle-particle and particle-wall interactions. These processes can be modelled and simulated with computationally intensive three-dimensional simulations. In this project, a combination of rigorous multiscale analytical and numerical techniques will be used to derive and calibrate faster and simple models for filtration and adsorption processes. Extensions to include additional phenomena, such as particle-particle interactions, electrostatic forces and electrochemical reactions will be also considered.

The proposed research will be particularly relevant for environmental applications such as groundwater remediation, as well as membrane technologies such as desalination. The development of new efficient, yet accurate models, for these applications is a crucial step towards the understanding and sustainable management of water resources of the planet. The project is part of a wider research effort that sees the collaboration of several UK and international academic partners, and industrial partners in the Environmental, Automotive, and Oil&Gas sector.

Summary: UK/EU students - Tuition Fees paid, and full Stipend at the RCUK rate, which is £14,553 per annum for 2017/18. There will also be some support available for you to claim for limited conference attendance. The scholarship length will be 3 or 3.5, depending on the qualifications and training needs of the successful applicant.

Eligibility/Entry Requirements: We require an enthusiastic graduate with a 1st class degree in Applied Mathematics (or other field such as Physics or Engineering, showing evidence of deep knowledge of continuum transport models and numerical methods), preferably at MMath/MSc level, or an equivalent overseas degree (in exceptional circumstances a 2:1 class degree, or equivalent, can be considered).

Apply: This studentship is available to start in January or September 2018 and remain open until it is filled. To apply please visit the University Of Nottingham application page: http://www.nottingham.ac.uk/pgstudy/apply

For any enquiries please email: matteo.icardi@nottingham.ac.uk

This studentship is open until filled. Early application is strongly encouraged.

School of Mathematical Sciences
PhD studentship in Mathematical Sciences

Quantifying uncertainties in multiphase flows through porous media

Supervised by Dr Matteo Icardi and Dr. Marco Iglesias

This project will be based at the University of Nottingham in the School of Mathematical Sciences in the group of Industrial and Applied Mathematics, and in collaboration with the GeoEnergy Research Centre.

Despite the recent significant developments in Digital Rock Physics (DRP), two-phase flows in complex pore geometries are still not fully predictable, understood, and quantitatively reproducible. This is due to a number of factors including imperfect physical models, insufficient mesh resolution, unknown parameters and pore heterogeneity. The qualitative and quantitative effects of these uncertainties have not been studied yet. In this project, we aim to develop a modelling and simulation workflow to quantify uncertainty and assess the validity of simplified multiphase flow models in digitalised porous media images. Deterministic and Monte-Carlo techniques, together with two-phase flow solvers, will be used to perform a global sensitivity analysis of the problem.

The project is part of a wider research effort that sees the collaboration of several UK and international academic partners, and industrial partners in the Automotive and Oil&Gas sector.

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School of Mathematical Sciences
PhD studentship in Mathematical Sciences

Data-driven coarse-graining and multiscale model reduction for ODEs and PDEs

Supervised by Dr Matteo Icardi and Dr. Donald Brown

This project will be based at the University of Nottingham in the School of Mathematical Sciences in the group of Industrial and Applied Mathematics.

Many theoretical tools have been recently developed to reduce the complexity of high-dimensional non-linear ODEs or three-dimensional PDEs in complex environments. These have now an enormous importance in computational chemistry, continuum mechanics, fluid dynamics, and dynamical systems in general. One of these bottom-up formal approaches is the Mori-Zwanzig projection formalism for dynamical systems. At the same time, also data-driven top-down methods, have been widely studied in machine learning and in numerical analysis. In this project, we aim to connect these theoretical and numerical tools to make them applicable for practical applications, such as the molecular dynamics simulation of complex molecule chains, or the relaxation to equilibrium of non-linear reaction-diffusion equations. In the first case, we can rely on the Hamiltonian structure of the full-resolution model, while the latter can be analysed, for example, through their discrete (particle- or mesh-based) counterparts, or through classical spectral analysis. The objective of this project is to develop and implement flexible numerical approaches to deal with the model reduction, multi-scale approximation, and/or coarse-graining of a limited number of model problems, by combining analytical derivations with numerical simulation data. Real-world applications in complex fluids and porous media will be considered.

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School of Mathematical Sciences
PhD studentship in Mathematical Sciences

Numerical upscaling and system identification for Lithium-Ion batteries

Supervised by Dr Matteo Icardi (Mathematics) and Dr. Alessandro Costabeber (Engineering)

This project will be based at the University of Nottingham in the School of Mathematical Sciences in the group of Industrial and Applied Mathematics, and in collaboration with the GeoEnergy Research Centre.

Rechargeable batteries and other energy storage technologies are key elements for reaching a sustainable carbon-free energy market. The increasing usage of batteries needs to be supported by more accurate and faster mathematical models to be integrated in control units of electric vehicles and other complex battery-operated future devices. Rechargeable battery models for control applications are typically defined by system identification techniques. Despite their computational simplicity, these models fail to capture the physical meaning and the dependence of the parameters on the underlying chemical-physical processes. Another mostly unresolved issue is the simulation of irreversible and complex non-linear phenomena such as fast (dis)charge and degradation

In this project, we aim to develop new mathematical techniques to develop simple and efficient reduced-order models, as an alternative to classical equivalent circuit models, to enable the fast, yet accurate, simulation of short and long-term behaviour of lithium-ion cells. Starting from the well-known porous electrode theory and PDE continuum models, we aim to derive simple differential equations that can retain the interesting features of the full model (e.g., polarisation, non-linearities). This will be integrated with data coming from both micro- and system-scale experimental data into via machine-learning approaches.

The project will focus on applications in the development of control units of electric vehicles, and it is part of a wider research effort that sees the collaboration of several UK and international academic partners, and industrial partners in the Automotive and Manufacturing sector.

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