Multiscale Modelling of Transport in Disordered Materials

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2nd supervisor: Dimitri Vvedensky (Physics, Imperial College London)
Collaborators: Robin Ball (Physics, University of Warwick)

Abstract
Transport in disordered systems is ubiquitous in science (e.g. electron transport in amorphous materials, diffusion on random lattices) with many practical applications (transport in biological systems, fuels cells, groundwater flow in aquifers). The common feature is that there is a field driving the flow (e.g. voltage in resistor networks). This field is random because of the underlying disorder in the material. In particularly complex cases (for example groundwater flow) this disorder can span many length scales from millimetres to tens of kilometres and is largely unknown in detail. All we have is the statistics of the disorder from which we need to predict the statistics of the flow rates. Furthermore, the physical nature of the driving force changes with length scale. To take the groundwater example again at the smallest scale flow of a contaminant is dominated by the interfacial tension between the fluid phases whereas at the larger scale flow is dominated by the density difference between the fluids.

This is hard to model numerically because of the wide range of length scales so a theoretical basis is required to relate transport at the micro-scale to that at the macro-scale. The renormalization group is ideally suited to this. Rather than the clumsy approach of using different numerical modelling schemes for different length scales the renormalization group gives a rational way of transforming transport coefficients between the length scales.

This project will focus on the transport in disordered porous media because the complexity of a wide range of length scales and different physical processes. There are also practical data available from industry. Although it should be emphasized that the methods are applicable to many other problems. The aim of this project is to derive physically robust methods that lead to properly coarse grained equations of motion appropriate to a particular statistical description of the heterogeneity. The methods used would be based on a newly formulated path integral for Darcy flow. This formulation was developed by a current CDT student\textsuperscript{4,5}. This has been developed primarily in one dimension with recent extensions to 2 and 3D and also to the flow of a single fluid rather than multiphase.

5. MJE Westbroek, GA Coche, PR King, DD Vvedensky, Pressure statistics from the path integral for Darcy flow through random porous media, *J Phys A* (in prep)
What is the multi-scale nature of the project?
The description of flow in porous media is inherently multiscale, as noted above. As the coarse-graining transformation is carried out, the effect of eliminated degrees of freedom is included in effective transport coefficients at large scales. The renormalisation group is the ideal way to transform between different length scales.

How do the expertises of the supervisors complement each other?
PRK has extensive experience in the multiscale modelling of flow in porous media and DDV has extensive experience in the statistical mechanics of coarse graining. RCB has worked with the principal supervisor (PRK) previously on applying the renormalisation group transformation to miscible flow in porous media.

Literature Review
Title: Application of renormalisation to upscaling flow in porous media

4. MI Morris and RC Ball, *Renormalization of miscible flow functions*, JPhys A 23, 4199
5. MJE Westbroek, GA Coche, PR King, DD Vvedensky, Evaluation of the path integral for flow through random porous media, *Physical Review E* 97 (4), 042119

MSc Project
There are two aspects for the prospective student to learn: the phenomenology of flow through porous media, and the methods of coarse graining used in statistical physics, mainly the renormalization group in real and momentum space. To gain familiarity with the problem at hand, a summer project would be to write a description of carrying out this program for a case study, for example, for miscible displacement which could build on previous renormalisation studies (M I Morris and R C Ball, *Renormalization of miscible flow functions*, JPhys A 23, 4199). This could be augmented by field data to examine a real example.