Matteo Icardi (University of Nottingham)

Upscaling challenges in advection-diffusion-reaction in porous media

Athough the basic understanding of the macroscopic limit of linear advection diffusion equations is well understood since the early developments of porous media theory (through, for example, homogenisation, and volume averaging), its extension to complex flow regimes is still currently an open question, even in presence of well-separated spatial scales. This is due to the presence of non-trivial microscopic equilibrium configurations (compared to the trivial constant solution obtained by standard periodic homogenisation), or of dynamic equilibrium configurations. For example, when dealing with fast surface reactions, high microscopic gradients can develop locally. Similarly, a conservative solute in the neighborhood of a concentration source (injection) undergoes a dynamic evolution of the local microscopic configuration in time and space before reaching the asymptotic self-similar profile. These are only two examples when the classical upscaling approaches fail, and effective macroscopic equations are often found either empirically or by resorting to generic random walk models.

In this talk, we present some (old and) new theoretical frameworks to overcome these limitations without the need of ad-hoc calibration or stochastic particle models. These generally involve solving more auxiliary local problems, and often computing local spectral properties (eigenvalues and eigenfunctions) of the underlying transport operators. In particular we will focus on i) an extension of the approach presented in [1] and [3] , considering a large-deviation (exponential) form for the concentration field, and on ii) model-order reduction based on projections from the full microscale formulation onto low-dimensional spaces, borrowing concepts from the finite element community (such as Hi-Mod ([4]), MsFEM, and VMM), and from statistical mechanics. New macroscopic equations are obtained for one or more macroscopic quantities, that can be seen as extended homogenised formulations. Applications of these techniques to the classical 2D Taylor dispersion in a channel and other heterogeneous periodic flows will be discussed.

[1] Allaire, G., Raphael, A. L. (2007). Homogenization of a convection-diffusion model with reaction in a porous medium. Comptes Rendus Mathematique, 344(8), 523–528.

[2] Battiato, I., Tartakovsky, D. M. (2011). Applicability regimes for macroscopic models of reactive transport in porous media. Journal of contaminant hydrology, 120, 18–26.

[3] Haynes, P. H., Vanneste, J. (2014). Dispersion in the large-deviation regime. Part 1: shear flows and periodic flows. Journal of Fluid Mechanics, 745, 321–350.

[4] Perotto, S. (2014). A survey of hierarchical model (Hi-Mod) reduction methods for elliptic problems. In Numerical simulations of coupled problems in engineering (pp. 217–241). Springer, Cham.

[5] Parish, E. J., Duraisamy, K. (2018). A Unified Framework for Multiscale Modeling Using Mori-Zwanzig and the Variational Multiscale Method. ArXiV preprint.