Proposition de sujet de stage M2 (2017-2018)

Time domain random walks for hydrodynamic transport in heterogeneous media : upscaling analysis

Random Walk methods have many advantages for simulating the transport of solute in low to highly heterogeneous porous media including its conceptual simplicity and easiness of implementation compared to more standard discretized methods such as finite volume, for example (see review by Noetinger et al., 2016). It has been presently developed for many areas of science, from biology and colloidal science to modern finance, including statistical physics, chemical engineering and geosciences for which it can be used for many applications in hydrology, energy extractive industry including shale gas production and geological storage of wastes and gases such as CO_2.

RW methods can be used for an extensive range of scales. For instance, at the laboratory scale, the recent advances in the 3D imaging techniques of rocks providing high-resolution pictures of the pore space associated with RW methods have proved to be very efficient (e.g. Gjetvaj et al., 2015). Furthermore RW method are intrinsically adapted to take into account (strongly variable) anomalous transport properties, preventing any classical description relying upon standard Darcy's law and Fickian Advection-Dispersion-Equation, encountered in moderate to high disordered media. RW methods can, for instance, represent "fractional derivative" and "non-local in time" transport equations accounting for memory effects over wide ranges of time (e.g. Gouze et al., 2008).

For 5 years, we have been developing a modeling platform using the Time Domain Random Walk (TDRW) approach, which is a space-discretized method that is well adapted to model spatially-defined heterogeneous media (Dentz et al., 2012; Russian et al., 2016). The method can be used indifferently at Stokes scale, taking into account Navier-Stokes flow in networks of pores or at Darcy scale. Recently, we have derived a general formulation of the TDRW approach to model the hydrodynamic transport of inert solutes in complex geometries and heterogeneous media (Russian et al., 2016). We demonstrated its formal equivalence with the discretized advection-dispersion equation and showed that the TDRW is equivalent to a continuous time random walk (CTRW) characterized by space-dependent transition times and transition probabilities, the transition times being exponentially distributed.

The aim of the proposed research M2 internship is to further develop the modeling platform and use it to investigate the pertinence of the approach for direct transport upscaling, which will give new insight into mass transfer in complex media ranging from pore networks to human tissue. The first task is to perform simulations for large 2D continuous systems (evaluating the possibility to extend to 3D) with increasing degree of heterogeneities and analyze the upscaled particle transition behavior in a stochastic approach. For instance, one of the questions to be answered is the relevance of the exponentially distributed transition time model when upscaling. Then, we will reiterate the simulations for vacuolar systems (network of heterogeneous connections) that mimic fracture networks and we will try to determine the relation between the particle transition statistics and some measurable topological properties of the network.

This work will require implementing a specific version of the TDRW optimized for massively parallel computation using large shared memory computer such as the 1500 Go RAM, 96 cores, machine we have in the team.

Student profile: applied mathematics or physicist with proved knowledge in hydrodynamics and scientific computing.

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