New efficient random walk particle tracking algorithms for transport in heterogeneous and discontinuous media

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Extended abstract

This study develops new Lagrangian particle methods for modeling flow and transport phenomena in complex porous media. Particle methods are well known for modeling transport problems[1][2]. They reduce or avoid some of the problems of Eulerian methods (e.g. instabilities, excessive diffusion, or oscillations that could lead to negative concentrations). Random Walk algorithms are used to model diffusion processes in the Lagrangian particle approach.

However, discontinuities and heterogeneities are difficult to treat, particularly discontinuous diffusion $D(\mathbf{x})$. The difficulties are different for the Eulerian PDE approach and for the Lagrangian Random Walk approach. In the literature on particle Random Walks, previous methods used to handle this problem could be characterized into two main types: the first one is called "Interpolation technique"[3] which smooths the discontinuity of the parameters, and therefore creates many cells near the interface that smooths it, so that it could be considered as a continuously variable rather than discontinuous coefficient. The second one is called "Partial reflection method", introduced by Uffink[4]. The discontinuous interface is taken into account by assigning probabilities for particle reflection and transmission across the interface [5] [6] [7]. One of the main drawbacks is the decrease in time step size required in order to converge to the expected solution. All these restrictions on the time step, lead to inefficient algorithms.

In this study, we propose a novel approach without any restrictions in the treatment of the particles jump and time step size. Moreover, the algorithm proposed here does not approach the solution but gives a semi-analytical solution with a maximum precision that depends solely on the number of particles.

The new method could be considered as a modified type of "Partial reflection method". The idea behind this new algorithm is inspired, from the analytical solution of the diffusion of an initial source in an infinite domain with an interface where the diffusion parameter is discontinuous. With the concept of negative mass particles, it allows to converge to the expected solution while keeping efficiency and robustness. In that configuration (see figure), it leads to the exact equation instead of approaching it. The method is combined with an asynchronous algorithm [8] that solves the overshoot problem [9].

Several test cases are investigated. For example, we show here the solution of the discontinuous diffusion problem at a given time (t_1) solved in one single time step, taking the time step equal to the final simulation time ($t_1 = \Delta t_1$). This method has been verified analytically, and validated in 1D by comparing the concentration profile obtained by the RWPT algorithm with the analytical solution (**Figure 1**).

Several other test cases with discontinuous transport parameters will be given and compared in 2D and 3D.

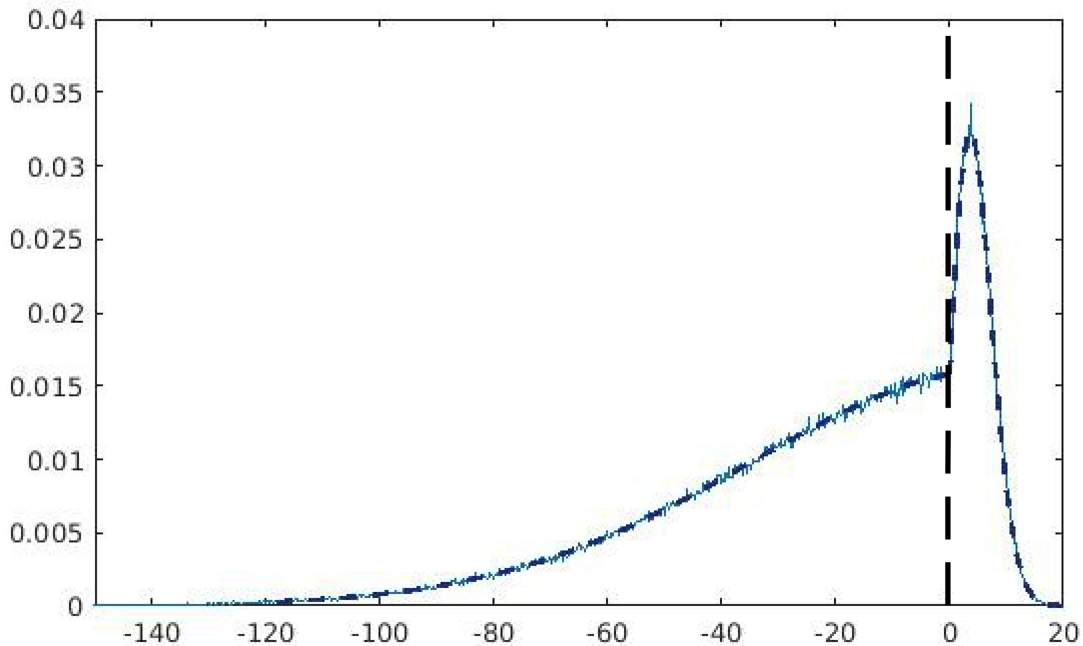

Figure 1: Comparison between analytical (PDE) and numerical (RWPM) concentration profile, for a 1D infinite domain problem with an initial Dirac mass at $x = x_0 = 1$ ("source"). The diffusion coefficient D(x) is discontinuous at x=0 (black dashed line). The dashed bold line is the analytical solution of the diffusion (PDE). The slightly fluctuating solid line is the result obtained by the RWPM with N = 1 Million initial particles. The diffusion contrast is $D_1/D_2 = 100$. This result was obtained by setting the time step equal to the final simulation time, for more efficiency and minimum calculation time.

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