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Global random walk algorithm for transport in media with discontinuous dispersion coefficients

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Random walk and grid-free particle tracking methods are valuable tools for simulating transport in highly heterogeneous porous media, when classical solutions to advection-dispersion equation often suffer from numerical diffusion. A long standing difficulty in particles methods is to account for discontinuous dispersion coefficients. Improvements are provided, for instance, by partially reflecting barriers and suitable spitting of time steps when particles cross the discontinuity interfaces. As an alternative, we propose a global random walk (GRW), consisting of large ensembles of particle tracking simulations projected on a regular grid. Hence, a single GRW simulation provides accurate concentration estimates at the grid sites. Since in GRW algorithms the particles starting at a grid site are spread globally, in a single numerical procedure, the computational costs are of the order of those for a single particle tracking trajectory. For purely dispersive displacements, we set the length of the particle's jump to a grid space step and model the variability of the dispersion coefficients through variable jump probabilities. In this way, no particle crosses the interface in a single time step and, unlike in grid-free particle tracking approaches, time splitting is not necessary. Instead of reflecting barriers, a continuity condition for the mass flux is also directly implemented in terms of jump probabilities. Advective transport can be further accounted for with a biased GRW, where advective displacements of the particles are modeled by biased jump probabilities.