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Evolution of the concentration PDF in random environments modeled by global random walk

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The evolution of the probability density function (PDF) of concentrations of chemical species transported in random environments is often modeled by ensembles of notional particles. The particles move in physical space along stochastic-Lagrangian trajectories governed by Ito equations, with drift coefficients given by the local values of the resolved velocity field and diffusion coefficients obtained by stochastic or space-filtering upscaling procedures. A general model for the sub-grid mixing also can be formulated as a system of Ito equations solving for trajectories in the composition space. The PDF is finally estimated by the number of particles in space-concentration control volumes. In spite of their efficiency, Lagrangian approaches suffer from two severe limitations. Since the particle trajectories are constructed sequentially, the demanded computing resources increase linearly with the number of particles. Moreover, the need to gather particles at the center of computational cells to perform the mixing step and to estimate statistical parameters, as well as the interpolation of various terms to particle positions, inevitably produce numerical diffusion in either particle-mesh or grid-free particle methods. To overcome these limitations, we introduce a global random walk method to solve the system of Ito equations in physical and composition spaces, which models the evolution of the random concentration's PDF. The algorithm consists of a superposition on a regular lattice of many weak Euler schemes for the set of Ito equations. Since all particles starting from a site of the space-concentration lattice are spread in a single numerical procedure, one obtains PDF estimates at the lattice sites at computational costs comparable with those for solving the system of Ito equations associated to a single particle. The new method avoids the limitations concerning the number of particles in Lagrangian approaches, completely removes the numerical diffusion, and speeds up the computation by orders of magnitude. The approach is illustrated for the transport of passive scalars in heterogeneous aquifers, with hydraulic conductivity modeled as a random field.