Karlstad Applied Analysis Seminar (2023)

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Random walk methods for reactive transport in porous media.

Abstract

Densities of computational particles moving along trajectories of Itô diffusion processes are often used to approximate solutions of parabolic and elliptic PDEs. Alternatively, particle densities can be approximated by using random walks on lattices, which provide weak solutions of the. Itô equation. In this approach, densities are readily obtained with a global random walk procedure (GRW), by using the binomially distributed numbers of random walk jumps to count the number of particles at every lattice site and time step. Since there is no need anymore to compute individual particle trajectories, GRW schemes increase the computational efficiency and the smoothness of the solution. Particularly, GRW schemes for reactive transport achieve a "microscopic" description of the process by using as many particles as the number of molecules involved in reactions.

In this seminar talk, I will first present the derivation of the GRW schemes for coupled nonlinear PDEs used in modeling reactive transport in porous media. Then, I will illustrate the approach for one- and two-dimensional biodegradation problems. Finally, I discuss the perspective of using microscopic descriptions by GRW simulations and space-time averages to model experimental concentration measurements.