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Locally optimal computation of complex reactions in RWPT

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Lagrangian approaches such as Random Walk Particle Tracking (RWPT) are an attractive alternative for modeling scalar transport in heterogeneous porous media. Unlike Eulerian approaches, these methods do not suffer from numerical dispersion or instabilities, and they are perfectly mass-conservative, among other advantages. However, incorporation of nonlinear reactions is challenging, since the concentrations are not readily available, and a link is needed between the particle distribution (representing only a random subsample of the solute) and the actual solute concentration distribution. Kernel Density Estimation (KDE) theory can be used to optimize the size of a kernel function to compute any kinds of nonlinear reactions. However, a kernel that is constant in space is suboptimal, due to the complexity of concentration distributions in heterogeneous porous media. In this work, we present a novel approach to define a locally adaptive kernel function, and show how local size and shape adaptability improve the accuracy of the density estimation and its convergence rate with respect to the number of numerical particles used in the simulation. This improvement is particularly important in extreme (especially low) density regions. Additionally, we show the positive impact that the approach has on the accuracy of reactive transport simulations in models of randomly heterogeneous porous media, as compared to the global KDE approach and also to non-KDE-based approaches.