Adaptive Local Kernels for Lagrangian Modeling of Reactive Transport

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Introduction

In recent years, a number of Lagrangian approaches [e.g. 1,2,3,4,5] have been proposed for the numerical solution of nonlinear reactive transport problems. In these approaches, reactions are driven by the interaction between numerical particles that represent either a volume of fluid or a mass of solute. This interaction is a function of the relative position of particles and can be derived mathematically by equipping each particle with a kernel function, sometimes referred to as the smoothing function. In some of these approaches, the choice of the kernel shape and size does not follow objective criteria, but is instead rather heuristic. On the other hand, some authors have proposed that the smoothing function should be derived from the dispersive process [e.g. 2,6].

Recently, we [7] proposed that the kernel should represent the probability density distribution of the actual particle location, and should be globally optimized by minimizing the Mean Integrated Squared Error (MISE) of the density estimation. By using the existing algorithms for the determination of a time-dependent globally optimal Kernel Density Estimator (KDE), it is possible to compute probabilities (or rates) of reaction of numerical particles to model simple bimolecular reactions [8] or kinetic reactions of any complexity involving two reactants [9].

The locally optimal kernel

Most research on KDE focuses on 1D distributions of limited complexity. However, solute concentration distributions in heterogeneous media exhibit complex features and variations in space and time (*Figure 1*). For this reason, the globally optimal kernel is often far from being locally optimal, in particular, in those parts of the domain with relative small particle densities that have a small impact on the MISE.

We present a novel approach to define an adaptive locally optimal kernel function that is not only time-dependent but also space-dependent. We derive the expressions for computing the locally optimal kernel in 2D and 3D, which require the estimation of some components of the distribution's Hessian matrix on a finite number of pilot points. To obtain them we use a global optimal kernel obtained from an existing algorithm [e.g. 10].

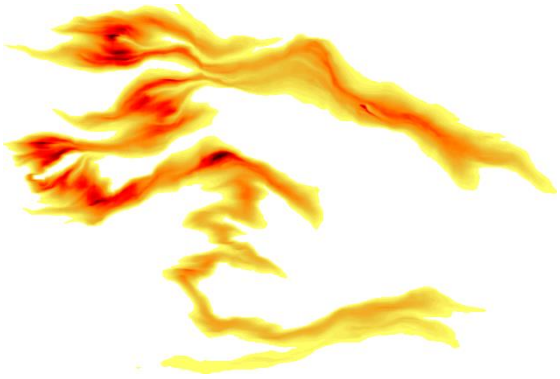

Figure 1: Mapped concentrations estimated at a given time from particle positions by KDE in an example RWPT simulation of conservative transport in a heterogeneous porous medium.

Three different levels of local adaptation (in terms of degrees of freedom of the kernel bandwidth matrices) are investigated: isotropic, diagonal and general bandwidth matrices. In the latter, we successfully incorporate information about the fluid velocities in the optimization process, and each local kernel has its own size, shape and orientation.

Results

We compare the presented local approaches against the existing global ones, in the context of a Random Walk Particle Tracking (RWPT) model of reactive transport through heterogeneous porous media. We show that the use of a locally adaptive kernel has a considerably positive impact in the accuracy of concentration estimations (particularly in low concentration areas) and consequently also on the accuracy of chemical reaction simulations. Convergence towards the correct solution occurs faster with respect to the number of particles when using the local kernel, hence this novel approach can be a valid alternative in order to avoid using an excessively high number of particles.

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