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Lagrangian Simulation of Reactive Transport: The Space-Time Adaptive Reaction Supports (STARS) Method

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Solute transport in fluids can be simulated with Lagrangian methods such as Random Walk Particle Tracking (RWPT). These methods are virtually free of numerical dispersion and instabilities, which makes them particularly well-suited to advection-dominated problems, and hence an attractive alternative to Eulerian approaches. However, incorporating nonlinear reactions in random walk models is not a straightforward task, since solute concentrations are not readily available. A simple approach for estimating the concentrations from particle positions would be to perform a simple binning, but this generates an estimation error. On the other hand, Kernel methods have been demonstrated to necessitate much lower particle numbers to reach the same degree of accuracy. A Gaussian kernel representing the dispersion Green's function in a time-step would virtually produce no over-smoothing bias, but, in many situations, it may require the use of prohibitive particle numbers for the solution to converge, especially for non-linear reaction systems. Thus, a wider, adaptive kernel that locally modifies its size and shape so as to optimally balance the noise and bias of the estimation can be a practical alternative. That is to assume that a particle is only a subsample of a much larger population and thus it represents a "cluster" of particles distributed over some support volume. Recent improvements in this area have led us to the development of the Space-Time Adaptive Reaction Supports (STARS) methodology, which can be used to generate density estimations efficiently, in 1, 2 or 3 dimensions, while accounting for the effect of boundary conditions. This methodology performs a pilot binning density estimation, and then smooths it using the local optimal kernel smoothers, whose size depends on x through the local particle distribution features, and evolves with time. With the link between particle positions and solute concentrations, we can implement all kinds of nonlinear reactions in random-walk models, including equilibrium reaction systems. Finally, we introduce the publicly available Matlab class STARS.m, which can be appended to a particle-based code to generate density estimations using the presented methodology.