Optimal reconstruction of non-symmetric travel time density distributions using a new kernel density estimator

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For typical solute transport applications using particle tracking algorithms, models are run with a limited number of particles and the estimation of the travel time density becomes an error-prone problem. Densities are however needed in groundwater applications, for instance to understand mixing, reactions and other type of phenomena occurring in the subsurface. Kernel density estimators (KDE) provide a convenient manner to reconstruct densities from travel time distributions and can be efficiently applied to reconstruct concentration gradients. KDE methods are based on an optimized smoothing algorithm, which improves the estimation of concentrations with respects to traditional methods such as histograms or other traditional approaches. A limitation of classical KDE methods is that numerical fluctuations occur in the regions where particles are scarce, which are on the other hand where concentration mass need to be more accurately estimated. We propose a new KDE method which automatically improves the estimation of particle travel time densities in the low-particle regions. Our solution allows one to obtain a better reconstruction of the density function without having to increase the number of particles and is especially good for estimating non-Fickian breakthrough curves with pronounced tailing.