Abstract Submitted
for the DFD16 Meeting of
The American Physical Society

Discrete kinetic and lattice Boltzmann formulations for reaction cross-diffusion systems and their hyperbolic extensions in chemotaxis

PAUL DELLAR, University of Oxford — We present discrete kinetic and lattice Boltzmann formulations for reaction cross-diffusion systems, as commonly used to model microbiological chemotaxis and macroscopic predator-prey interactions, and their hyperbolic extensions with fluid-like persistence terms. For example, the canonical Patlak–Keller–Segal model for chemotaxis involves a flux of cells up the gradient of a chemical secreted by the cells, in addition to the usual down-gradient diffusive fluxes. Existing lattice Boltzmann approaches for such systems use finite difference approximations to compute the flux of cells due to the chemical gradient. The resulting coupling between, and necessary synchronisation of the evolution of, adjacent grid points greatly complicates boundary conditions, and efficient implementation on graphical processing units (GPUs). We present a kinetic formulation using cross-collisions between bases of moments for the two sets of distribution functions to couple the fluxes of the two species, from which we construct lattice Boltzmann algorithms using second-order Strang splitting. We demonstrate an efficient GPU implementation, and verify second-order spatial convergence towards spectral solutions for benchmark problems such as the finite-time blow-up in the Patlak–Keller–Segal model.

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Date submitted: 31 Jul 2016 Electronic form version 1.4