Simulating the dynamics of a single polymer chain in solution: Lattice Boltzmann vs Brownian Dynamics

Burkhard Dünweg[1,2], Tri T. Pham[2], Ulf D. Schiller[1], J. Ravi Prakash[2]

[1] Max Planck Institute for Polymer Research, Mainz, Germany
[2] Department of Chemical Engineering
Monash University, Clayton, Victoria, Australia

Abstract

One possible way of simulating the dynamics of Brownian particles in solution is via dissipative coupling of such particles to a Lattice Boltzmann background fluid, and adding Langevin noise to both parts. This method however competes with the established approach of implementing a hydrodynamic interaction tensor in a Brownian Dynamics simulation. After a brief introduction into both methods, a benchmark calculation is presented, in which the dynamics of a single flexible polymer chain in good solvent is studied. Very good agreement between both methods is found after proper extrapolation to the infinite-volume limit, provided that the fluid is thermalized with respect to all non-conserved degrees of freedom, i.e. with respect to both the stresses and the kinetic modes. For this particular system, Brownian Dynamics is found to be computationally more efficient. However, it is argued that this situation is reversed if one rather studies a semidilute system.

See also: Tri T. Pham, Ulf D. Schiller, J. Ravi Prakash, and B. Dünweg, J. Chem. Phys. 131, 164114 (2009).