Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A particle-in-mesh method for Brownian Dynamics simulation of many-particle systems with hydrodynamics interactions in a confined geometry XUJUN ZHAO, Argonne National Laboratory , JUAN HERNANDEZ-ORTIZ, Univ. Nacional de Colombia, DMITRY KARPEYEV, Argonne National Laboratory , JUAN DE PABLO, University of Chicago, BARRY SMITH, Argonne National Laboratory — In this work, we present an efficient parallel particle-in-mesh method for Brownian Dynamics simulations of many-particle systems confined in micro- and nano-fluidic devices. A general geometry Ewald-like method (GGEM) combined with finite element method is used to account for the hydrodynamic interaction. A fast parallel Krylov-type iterative solver with hybrid preconditioning techniques is developed for solving the large sparse systems of equations arising from finite element discretization of the Stokes equations. In addition, the current computer code is developed based on PETSc, a scalable library of numerical algorithms developed at Argonne, SLEPc - Scalable Library for Eigenvalue Problem Computations, and libMesh, a finite element library for numerical solution of PDEs built on top of PETSc, which allows for direct simulation of large scale systems with arbitrary confined geometries. This scheme is applied to Brownian dynamics simulations of flowing confined polymer solutions and colloidal dispersions in micro-fluid channels. The effects of hydrodynamics interactions and geometric confinement on the migration phenomena are illustrated.

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Date submitted: 06 Nov 2015 Electronic form version 1.4