Abstract Submitted
for the DFD12 Meeting of
The American Physical Society

Multiscale simulation of electroosmotic flows LIN GUO, MARK ROBBINS, Johns Hopkins University, SHIYI CHEN, Johns Hopkins University and Peking University, JIN LIU, Washington State University — We develop an efficient hybrid multiscale method for simulating nano-scale electroosmotic flow based on spatial "domain decomposition" [1]. Molecular dynamics (MD) is used in the near wall region where atomistic details are important. AmultigridParticle-Particle Particle-Mesh (PPPM) method [2] is used to calculate the long-range Coulombic interaction between charged ions. Continuum (incompressible Navier-Stokes) equations for the solvent are solved in the bulk region, reducing the computational cost substantially. A discrete description of ions is retained in the continuum region because of the low density of ions and the long-range of electrostatic interactions. Langevin dynamics is used to model the Brownian motion of these ions in the implicit solvent. The fully atomistic and continuum descriptions are coupled through "constrained dynamics" [1] in an overlap region. Flux of charged and solvent particles between continuum and MD regions is included. Simulation results for different channel sizes are provided. To benchmark this multiscale scheme, we compare results with pure MD simulations.

[1] X. B. Nie, S. Y. Chen, W. N. E, and M. O. Robbins, J. Fluid Mech., 500:55–64, 2004.
[2] J. Liu, M. R. Wang, S. Y. Chen, and M. O. Robbins, J. Comput. Phys., 229:7834-7847, 2010.

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Date submitted: 10 Aug 2012 Electronic form version 1.4