Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Coupling Fluctuating Hydrodynamics with Molecular Dynamics at the Nanoscale NIKOLAOS VOULGARAKIS, JHIH-WEI CHU, Department of Chemical and Biomolecular Engineering, University of California, Berkeley — Hydrodynamic fluctuations and solvation interactions are essential driving forces of transport phenomena in the micrometer to nanometer regime, including inter- and intra-cellular flows and flows in nanofabricated devices. Although all-atom molecular dynamics (MD) simulations can be used to model molecular fluids, the accessible time- and length-scales are severely limited. Since most of computational cost for MD simulations comes from the represetion of solvent molecules, a possible solution to this limitation is to model fluids with fluctuating hydrodynamics (FHD). While this approach reduces the computational time of MD simulations by three orders of magnitude, an accurate protocol to couple FHD with MD is still necessary. In this work we present a new methodology that couples FHD with MD by allowing the fluctuating fields to directly interact with particles through repulsive, attractive, and dissipating/fluctuating forces without introducing new degrees of freedom or boundary conditions. Numerical results show that solvation energy and diffusion dynamics are correctly described within our framework. Simulations on the collapse of two hydrophobic particles are also presented.

Nikolaos Voulgarakis
Department of Chemical and Biomolecular Engineering,
University of California, Berkeley

Date submitted: 23 Nov 2010 Electronic form version 1.4