Abstract Submitted for the MAR14 Meeting of The American Physical Society

Lipid Bilayer Membrane Elasticity and Hydrodynamics: Insights from Dynamic Implicit-Solvent Coarse-Grained Models PAUL ATZBERGER, University of California Santa Barbara — Lipid bilayer membranes have been widely studied using fully atomistic molecular dynamics and continuum mechanics descriptions. To bridge this gap many mesoscale implicit-solvent models have been developed to capture at equilibrium essential features of lipid bilayer membrane formation and internal structure, while at the same time providing enough simplification in simulations to allow access to large spatial scales. To study dynamic processes in such implicit solvent models requires further advances to account for important kinetic effects mediated by the solvent. We discuss our recent progress on developing thermostats for dynamic processes based on continuum fluctuating hydrodynamics for implicit-solvent coarse-grained models of lipid bilayer membranes. We present results for vesicle bilayers making comparisons with explicit solvent simulations and continuum theory.

Paul Atzberger University of California Santa Barbara

Date submitted: 18 Nov 2013 Electronic form version 1.4