Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Toward a multi-scale simulation of lipid bilayer systems TAISUKE SUGII, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo —
In numerical simulations of lipid bilayer systems, it has become important to treat the membrane molecules (e.g., lipids, proteins, and drug molecules) explicitly for designing medical drugs and for developing drug delivery systems. However, it is difficult to apply straightforwardly a microscopic simulation technique such as the molecular dynamics method to the large-scale bilayer systems, because the length and the time scales of these systems are very large compared to the scales of the molecules. The authors take two approaches for this problem. First, we use the dissipative particle dynamics method and the coarse grained molecular dynamics method in addition to the standard molecular dynamics method. The results are compared with the molecular-dynamics results and experimental data. Secondly we use a molecular dynamics and continuum hybrid simulation method. In this method, the region near the membrane is computed by an atomistic-simulation method and the solvent region is computed by a continuum-simulation method. (In our study, the coarse grained molecular dynamics was used for the atomistic region.) The validity and availability of this later approach will be discussed.

Taisuke Sugii
The University of Tokyo

Date submitted: 29 Nov 2005 Electronic form version 1.4