Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

**Simulating ligand receptor binding at a membrane interface with graphics processing accelerated coarse-grained molecular dynamics** SHARON M. LOVERDE, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, DAVID N. LEBARD, Department of Chemistry, Temple University, ZHENGYU MA, Penn Institute for Immunology, University of Pennsylvania, MICHAEL L. KLEIN, Department of Chemistry, Temple University, DENNIS E. DISCHER, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — Motivated by a deeper understanding of the immunological synapse, we develop a molecular-based model to understand receptor-polymer/ligand binding at a membrane interface. We examine the case of weak ligand binding in the limit of confined polymer chains as a function of chain length, binding constant, and system size. We utilize a coarse-grained (CG) model of poly(ethylene oxide) and dimyristoylphosphatidylcholine (DMPC) previously developed by the Klein group and mimic weak binding with a sticky potential. This work employs graphics processing units (GPU) to accelerate the CG-MD simulations, where each simulation is run with multiple random-walker replicas to enhance sampling and facilitate statistical convergence of physical observables. Our results demonstrate that such an aggressive combination of GPU acceleration with CG modeling can yield accurate and precise data on polymer-DMPC binding, and, more importantly, hints at the mechanism behind empirical data of polymer binding to a T-cell receptor protein.

Sharon Loverde
University of Pennsylvania

Date submitted: 10 Nov 2011 Electronic form version 1.4