Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Solvent-Shift Monte Carlo: A cluster algorithm for solvated atomistic and coarse-grained systems DAVID EARL, CHRISTOPHER HIXSON, JAMES BENIGNI, Department of Chemistry, University of Pittsburgh — We present a cluster algorithm for the efficient simulation of solvated molecules that we term solvent-shift Monte Carlo (SSMC). The algorithm involves a conformational change in a solvated solute molecule of interest, followed by a geometrical rotation of solvent particles. The method satisfies detailed balance and can be applied to existing schemes to sample conformational space, where an axis or plane of rotation can be defined. We demonstrate that the algorithm significantly enhances the sampling of phase space in solvated systems, and may be easily combined with other advanced sampling techniques such as parallel tempering.

David Earl
University of Pittsburgh

Date submitted: 20 Nov 2008 Electronic form version 1.4