Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A statistical estimation of the precision of reweighting-based simulations DANIAL SABRI DASHTI, Quantum Theory Project and Physics Department, University of Florida, ADRIAN E. ROITBERG, Quantum Theory Project, University of Florida — Reweighting a sampled configuration plays a central role in decreasing the computational cost of a simulation involving ergodic and semi-ergodic systems and is the base of all biased sampling methods. A very simple application of this method is reweighting a primary ensemble, usually generated by a computationally cheap Hamiltonian, to a target ensemble, typically a more expensive Hamiltonian. However, the precision can be strongly affected by the distribution of the Hamiltonians' difference in each bin of conformation distribution. Theoretically, one should sample forever to have a complete distribution of energy in the ensemble, but sampling in energy space is much faster than sampling in conformation space. Using this idea and taking advantage of the Gaussian nature of the energy distribution, we study a way to make a good estimate of error in reweighting histogram procedures before running a long simulation on the system. We are applying these ideas on two polypeptide chains, ala 10 and fs21, to see how they work practically.

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Date submitted: 23 Nov 2009 Electronic form version 1.4