Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Optimized Nested Markov Chain Monte Carlo Sampling: Theory JOSHUA COE, Theoretical Division, Los Alamos National Lab, THOMAS D. SEWELL, University of Missouri at Columbia, M. SAM SHAW, Theoretical Division, Los Alamos National Lab — Metropolis Monte Carlo sampling of a reference potential is used to build a Markov chain in the isothermal-isobaric ensemble. At the endpoints of the chain, the energy is reevaluated at a different level of approximation (the "full" energy) and a composite move encompassing all of the intervening steps is accepted on the basis of a modified Metropolis criterion. By manipulating the thermodynamic variables characterizing the reference system we maximize the average acceptance probability of composite moves, lengthening significantly the random walk made between consecutive evaluations of the full potential at a fixed acceptance probability. This provides maximally decorrelated samples of the full potential, thereby lowering the total number required to build ensemble averages of a given variance. The efficiency of the method is illustrated using model potentials appropriate to molecular fluids at high pressure. Implications for ab initio or density functional theory (DFT) treatment are discussed.

Joshua Coe
Theoretical Division, Los Alamos National Lab

Date submitted: 19 Feb 2009 Electronic form version 1.4