

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Acceleration of Markov Chain Monte Carlo Simulations through Sequential Updating RUICHAO REN, GERASSIMOS ORKOULAS, University of California, Los Angeles — Strict detailed balance is not necessary for Markov chain Monte Carlo simulations to converge to the correct equilibrium distribution. In this work, we propose a new algorithm that only satisfies the weaker balance condition. The new algorithm is based on sequential updating moves with a small fraction of randomness to eliminate possible oscillatory effects. We prove analytically that the new algorithm identifies the correct equilibrium distribution. In addition, based on the properties of the diagonal elements of the underlying transition matrices, we demonstrate that the new algorithm converges faster than the Metropolis algorithm with strict detailed balance. We illustrate the efficiency of the new algorithm on the two- dimensional Ising model. The sequential update algorithm also compares well with multispin-based Monte Carlo techniques. The new method, however, is very general and can be readily extended to off-lattice continuum systems in various ensembles (canonical and grand canonical) with minor modifications. Simulation results on hard-spheres, square-well, and Lennard- Jones fluids indicate that the new method is more efficient in reducing autocorrelation times than conventional Metropolis- type of algorithms in canonical and grand canonical ensembles. Regarding off-lattice continuum fluids, autocorrelation time reduction is more substantial at higher densities due to the sequential nature of the Monte Carlo moves.

Gerassimos Orkoulas
University of California, Los Angeles

Date submitted: 04 Dec 2005

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