# Sequential Updating Algorithms in Monte Carlo Simulations of Thermophysical Fluid Properties

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Strict detailed balance is not necessary for Markov chain Monte Carlo simulations to converge to the correct equilibrium distribution. Recently, we proposed 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 behavior. We prove analytically that the new algorithm identifies the correct equilibrium distribution of states. Based on the properties of the diagonal elements of the transition matrices, we prove that the new algorithm is more "mobile" than the standard Metropolis algorithm. We also demonstrate that the new algorithm converges faster than the Metropolis algorithm with strict detailed balance. We first illustrate the efficiency of the new algorithm on the two-dimensional Ising model. The sequential updating algorithm 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, grand canonical, semi-grand) 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 the conventional Metropolis-type 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 techniques. The new methodologies are well-suited for fluid-fluid and fluid-solid phase coexistence calculations.