475d Detailed Balance and Markov Chain Monte Carlo Simulation with Sequential Updating

Ruichao Ren and Gerassimos Orkoulas

In this work, we consider Monte Carlo simulations with sequential updating moves. Although detailed balance is satisfied in most Monte Carlo simulations, we show that for the case of Monte Carlo simulations with sequential updating, the underlying Markov chain will eventually converge and preserve the desired distribution without strictly satisfying detailed balance. We also show that Monte Carlo simulations with sequential updating moves converge faster to the desired equilibrium distribution and yield better sampling statistics than Monte Carlo simulations that satisfy detailed balance. We corroborate our findings by performing Monte Carlo simulations for the Ising model and the Lennard-Jones fluid. Remarkably, sequential updating is particularly advantageous than its random updating counterpart in Monte Carlo simulations of large, near-critical systems.