Optimizing Monte Carlo Simulations by Using Transition Probability Data

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Conventional Monte Carlo simulation often undergoes quasi-ergodicity issues, that is, high free-energy barriers impede a proper sampling of phase space. In contrast, Flat Histogram simulations are usually able to overcome these barriers by uniformly sampling a predefined range of a convenient order parameter. Recently, Trebst et al. [Physical Review E 70, 046701, 2004] have shown that producing faster round trips is better than sampling such range uniformly. Their method compares the number of visits to each parameter value in the two stages of a round trip (up and down) in order to resolve the optimal sampling weights and calculate the system's density of states. In the present work, we develop a way of performing both tasks by means of the transition rates among distinct parameter values. For this, we consider that the two stages are separate Markov processes and determine their stationary probability distributions. In addition, we resort to the theory of absorbing Markov chains to recalculate the round trip time, obtaining a good agreement with the actual value achieved in the simulation. This permits us to estimate the round trip time that different weights would cause without having to run a new simulation. We take advantage of this possibility to obtain sampling weights using a numerical optimization procedure instead of using the approximate analytical procedure of Trebst et al. Finally, we apply this methodology to speed up simulations of lattice model proteins specially designed to exhibit folding transition.