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Wang-Landau and stochastic approximation Monte Carlo for semi-flexible polymer chains

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Abstract

We present a comparison of the performance, relative strengths and relative weaknesses of standard Wang-Landau Monte Carlo simulations and Stochastic Approximation Monte Carlo simulations applied to semi-flexible single polymer chains.
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1. Introduction

Ever since Wang and Landau suggested a new type of flat histogram Monte Carlo method, the now so-called Wang-Landau Monte Carlo (WLMC) method Wang and Landau (2001a,b), to determine the density of states of a given system, the method has found widespread applications and undergone significant practical development in its implementations. Important for our purposes here are applications to determine the density of states of single polymer chains Wüst el al. (2011); Rampf et al. (2005); Rampf el al. (2006); Paul et al. (2007); Taylor el al. (2009, 2013a,b); Seaton et al. (2013) for which the method is now an alternative to Multicanonical simulations Bachmann and Janke (2003, 2004), and sometimes both methods are used in conjunction. Having the density of states, $g(E)$, available, one can obtain the microcanonical entropy, $S(E) = \ln g(E)$ or the canonical partition function, $Z(T) = \sum_E g(E) \exp\{-\beta E\}$ with $\beta = 1/k_B T$. Both, $g(E)$, and its Laplace transform, $Z(T)$, contain the complete information on the thermodynamics of the system.

The WLMC method starts from the observation, that if one knew the density of states, one could generate a random walk over the possible energy values by a Monte Carlo simulation of an unbiased stochastic process in configuration space, where starting from a micro-state, x, a new state, x', is accepted with a probability $\min[1, g(E(x))/g(E(x'))]$. As the correct $g(E)$ is to be determined, the idea is to start from an unbiased guess, $g(E, t = 0) = 1$, and update this

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guess by some modification factor $g(E(x'),t) = f(t)g(E(x'),t)$ when a state x' occurs in the generated time series. The modification factor is set to $f(0) = e$ at the start. For each fixed value of f one samples a visitation histogram, $h(E)$, to the possible energies, and when this histogram is "flat" enough at some time t_n, f is reduced in an exponential fashion, $f(t_n) = f(t_n + 1)^{1/2}$ and $h(E)$ is reset to zero for all energy values. This is iterated until $\ln(f(t)) < \varepsilon$ with $\varepsilon = 10^{-8}$ in many applications of the method to polymer systems.

While the method has shown enormous practical applicability, it was found early on Lee et al. (2006); Belardinelli and Pereira (2007a,b); Swetnam and Allen (2010) and analyzed in detail Belardinelli and Pereira (2007b) that the error in the resulting $g(E)$ actually did not go to zero with increased simulation effort, but was actually bounded and of order $\sqrt{f_{\text{final}}}$. In Belardinelli and Pereira (2007b) it was shown that in order for the error to go to zero, the following quantity

$$\ln[g(e,t)] = \sum_{i=1}^{t} [H(E,i) - H(E,i-1)] f_i \tag{1}$$

where $H(E,i)$ is the cumulative histogram up to refinement level i of the modification factor has to diverge. If f is reduced in an exponential way like in the original WLMC method, this sum converges and thus the achievable error is bounded from below. The authors of Belardinelli and Pereira (2007a,b) suggested to use a variation of f which asymptotically goes like $1/t$ to create an algorithm which does not suffer from this problem. In an initial phase, f is modified according to the original WLMC idea until $f < 1/t$ and from then on it is reduced as $1/t$, where t is Monte Carlo time.

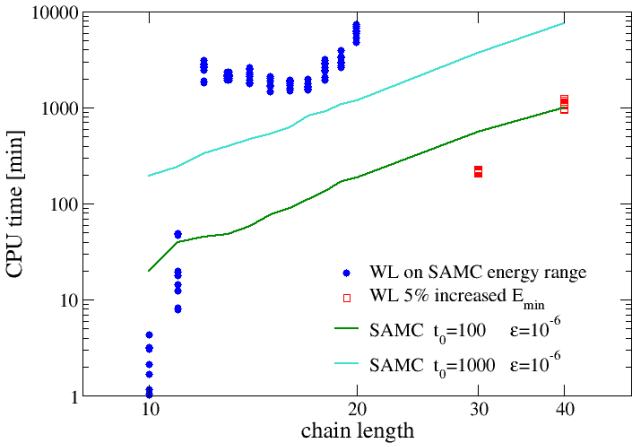

Fig. 1. CPU times for WLMC runs (8 runs per chain length) blue circles and WLMC runs with increased energy minimum (red squares). The lines are times for SAMC runs using the parameters indicated in the legend. All results are for flexible chains.

One objection often raised against WLMC that is not resolved by this change of f-update is the fact, that the Monte Carlo simulation does not fulfill detailed balance, as long as $g(E)$ keeps being modified and attempts have been made to prove convergence of the method as a Markov Chain Monte Carlo (MCMC) method in some larger configuration/parameter space Zhou and Batt (2005). However, Liang et al. Liang (2006); Liang et al. (2007) proved convergence of the method from a completely different perspective. Consider the task to find a function $u(x)$ which generates a random walk over the possible energy values when used as the acceptance probability in the master equation

$$p(x,t+1) = p(x,t) + \sum_{x'} w_0 \min\left(1, \frac{u(x')}{u(x)}\right) p(x',t) - \sum_{x'} w_0 \min\left(1, \frac{u(x)}{u(x')}\right) p(x,t)\,, \tag{2}$$

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