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# Stochastic approximation Monte Carlo and Wang–Landau Monte Carlo applied to a continuum polymer model

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ABSTRACT

We discuss Stochastic Approximation Monte Carlo (SAMC) simulations, and Wang–Landau Monte Carlo (WLMC) simulations as one form of SAMC simulations, in an application to determine the density of states of a class of continuum polymer models. WLMC has been established in the literature as a powerful tool to determine the density of states of polymer models, but it has also been established that not all versions of WLMC really converge to the desired density of states. Convergence of SAMC simulations has been established in the mathematical literature and discussing WLMC as a special case of SAMC brings a clearer perspective to the properties of WLMC. On the other hand, practical convergence of SAMC simulations with a fixed simulation effort needs to be established for given physical problems and, for practical applications, the relative efficiency and accuracy of the two approaches need to be compared.



## 1. Introduction

Wang–Landau Monte Carlo simulations belong to the broader class of flat-histogram Monte Carlo simulations aimed at obtaining an estimate of the density of states of a system. They were first applied to spin models [1,2] but their use was soon extended to polymer models [3–9]. In the last ten years WLMC has been shown to be a very powerful tool for the determination of the density of states of polymer models, see, e.g., [10–16] or reviews in [17–19], comparable to multi-canonical simulation approaches [20–22]. The convergence properties of the original formulation of WLMC has been an issue of controversy [23,24] and simulations clearly pointed to a saturation of the final error [25] irrespective of the simulation effort employed. This has led to the suggestion of a modification of the original method [26,27] which was shown to converge in the selected applications. However, it has been pointed out [28] that the practical convergence properties also of this version of WLMC may be strongly dependent on the physical model it is applied to.

In parallel to much of this development, Stochastic Approximation Monte Carlo (SAMC) has been formulated [29,30] in the context of stochastic optimization problems. Liang et al. [30] showed that WLMC could be seen as a version of SAMC and using the mathematical background of stochastic approximation methods they proved the convergence of SAMC. Understanding the necessary conditions for this convergence also clarified why the modified WLMC [26,27] converged, whereas the original version [1,2] yielded an excellent (and adjustable) approximation to the density of states, but did not strictly speaking converge.

We will discuss in the next section the theoretical background of the SAMC and WLMC ideas and discuss in which way WLMC can be seen as a version of SAMC. This discussion will also point out strong and weak points for the practical use of both methods. An abridged first comparison of the two methods has been presented in [31]. In Section 3 we will introduce the model for which both methods will then be compared with respect to their practical usefulness. Section 4 will then compare the two methods concerning quality of convergence with a given simulation time effort and discuss the tunability of the SAMC method, which has not been systematically analyzed for applications to physics problems so far, by suitable choice of its free parameters. Finally, Section 5 will present our conclusions.

## 2. Theoretical background

The idea of the WLMC method [1,2] is that an unbiased random walk over micro-states (random walk in configuration space) will visit every admissible energy value of a Hamiltonian defined on this configuration space proportional to the number of micro-states, $g(E)$, with that energy (or the measure of the set of points in configuration space having an energy in the interval $[E, E + dE]$

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for continuous ranges of energies and states). The quantity, $g(E)$, is the density of states of the model. When one accepts a suggested transition between micro-states $x'$ with energy $E'$ and $x$ with energy $E$ with a modified Metropolis probability $\min(1, g(E')/g(E))$, a random walk over the range of admissible energies will be created. Since $g(E)$ is not known but the target of the simulation, one determines it iteratively. At the beginning of the simulation one starts from the unbiased assumption $g(E) = 1\,\forall\, E$, i.e., $\ln[g(E)] = 0\,\forall E$ (since $g(E)$ varies over hundreds of orders of magnitude, one typically works with $\ln[g(E)] = S(E)$, where $S(E)$ is the micro-canonical entropy). One also introduces a histogram of visits, $H(E)$, to each energy state and a modification factor, $f$, which is typically set to $f = e$ (Euler's constant) as a start. During the WLMC simulation one monitors the flatness of $H(E)$ and when $|H(E)/\overline{H(E)} - 1| < 1 - c\,\forall\, E$, where $\overline{H(E)}$ is the average visitation to all energy values, one changes $f \to \sqrt{f}$ and resets $H(E) = 0\,\forall\, E$. The constant $c$ is typically taken as $c \geq 0.8$. An update at level $n$ of the modification factor then reads

$$\ln[g(E)] = \ln[g(E)] + 2^{-n} \qquad (1)$$
$$H(E) = H(E) + 1.$$

Experience [11,12] shows that for continuum polymer models this has to be continued until $2^{-n}$ is of the order $10^{-7} - 10^{-8}$, i.e., up to $n = 23 - 26$. The resulting $\ln[g(E)] = S(E)$ is only determined up to a constant arbitrary shift factor. We want to note two properties here for future reference which are both connected to the use of a visitation histogram.

- The run time of the algorithm is not predictable as the times when the flatness criterion is fulfilled are stochastic.
- One has to know the admissible energy range for the model at the outset (or determine it from pre-runs) and work only in this energy range, as otherwise the flatness criterion would never be fulfilled.

We also note, that for this original choice of variation of the modification factor (which is exponential as a function of simulation time) it can be shown that the method approximates the true density of states but the final error is bounded from below, irrespective of the CPU time effort. The value of the bound can be reduced by increasing $c$ towards one, but at an unsustainable cost in CPU time. This led to the suggestion [26,27] to only use the original version up to a certain level $n_0$ and then change to $\ln f \sim 1/t$, where $t$ is the simulation time. We discuss the reason for this in the context of the SAMC method.

The mathematical foundations of SAMC were discussed by Liang et al. in two publications [29,30]. We will present the method here in a notation adapted to our above discussion of WLMC and ignoring mathematical special cases which are not relevant for our discussion in Section 4. Assume an energy interval $[E_{\min}, E_{\max}]$ which can be larger than the admissible energy range of the model system, specifically one can choose $E_{\min} < E_{gs}$, where $E_{gs}$ is the ground state of the model. We further assume that we have a set of $M$ discrete energy states, either because they are intrinsic to the model or because we have performed a numerically necessary binning of adjacent energies when the model has a continuous variation of admissible energies. Let $\gamma_t$ now denote the modification factor for our estimate for the logarithm of the density of states, which we denote by $\ln[\tilde{g}(E)]$. We furthermore introduce a desired sampling probability $p^*(E)$ for the energies in $[E_{\min}, E_{\max}]$ with

$$\sum_{E_{\min}}^{E_{\max}} p^*(E) = 1. \qquad (2)$$

The SAMC update then is

$$\ln[\tilde{g}(E)] = \ln[\tilde{g}(E)] + \gamma_t \left(\delta_{E,E_{\text{new}}} - p^*(E)\right), \qquad (3)$$

so $p^*(E)$ is subtracted in each update for all $E$, and only for the new energy, $E_{\text{new}}$, accepted in the Monte Carlo procedure, the modification factor $\gamma_t$ is added to $\ln[\tilde{g}(E_{\text{new}})]$. The following two necessary conditions exist for this method to converge:

$$\sum_{t=1}^{\infty} \gamma_t = \infty \qquad (4)$$

$$\sum_{t=1}^{\infty} \gamma_t^{\nu} < \infty \quad \text{for some } \nu \in (1, 2). \qquad (5)$$

The first of these conditions is violated by the original update version [1,2] of WLMC which explains its lack of convergence, but it is fulfilled in the modified update [26,27]. The SAMC update scheme converges in the following form

$$\ln[\tilde{g}(E)] \to \ln[g(E)] + C - \ln[p^*(E) + \Phi] \quad E \in \{E\}_{\text{adm}} \qquad (6)$$

$$\ln[\tilde{g}(E)] \to 0 \quad E \notin \{E\}_{\text{adm}}, \qquad (7)$$

where $\{E\}_{\text{adm}}$ is the set of admissible energy values of the model and $C$ is an undetermined constant. If we let $M_0$ be the number of energy states in the chosen energy interval which are not admissible energy states of the model, then

$$\Phi = \frac{1}{M - M_0} \sum_{E \notin \{E\}_{\text{adm}}} p^*(E). \qquad (8)$$

The sampling frequency we introduced, $p^*(E)$, defines the visitation probability of the different energy states when the procedure converges, i.e., one should have

$$\frac{H(E)}{\sum_E H(E)} \to p^*(E) \quad E \in \{E\}_{\text{adm}}. \qquad (9)$$

Analytically, the choice of $p^*(E)$ is arbitrary, the method converges for all choices in the limit of infinite simulation time. Numerically, however, different choices may prove more or less efficient. We will discuss two choices in the results section. To make contact with the WLMC method we have to consider a flat sampling of the energy interval, $p^*(E) = 1/M$. Then we have from Eq. (6)

$$\ln[\tilde{g}(E)] \to \ln[g(E)] + C' \qquad (10)$$

where we have subsumed all constants on the right side into one constant $C'$. Since $\ln[g(E)]$ can only be determined up to an unknown constant anyhow, this is the approximation idea of the WLMC method. A discussion of the convergence of WLMC therefore should not be performed within the context of Markov chain Monte Carlo methods and detailed balance conditions, but as a special case of SAMC.

In our simulations, we will employ a modification factor similar to the one suggested by Liang et al. [29,30]

$$\gamma_t = \gamma_0 \frac{t_0}{\max(t_0, t)}, \qquad (11)$$

where we have introduced a scale factor $\gamma_0$ compared to their suggestion. This modification factor has a $1/t$ time dependence for late times and therefore leads to a convergent algorithm. As a final note, let us state here that for SAMC we have:

- The run time is predictable from the choice of parameters and Monte Carlo moves.
- The admissible energy range of the model does not need to be known before hand.