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Efficient simulated tempering with approximated weights: Applications to first-order phase transitions

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ABSTRACT

Simulated tempering (ST) has attracted a great deal of attention in the last years, due to its capability to allow systems with complex dynamics to escape from regions separated by large entropic barriers. However its performance is strongly dependent on basic ingredients, such as the choice of the set of temperatures and their associated weights. Since the weight evaluations are not trivial tasks, an alternative approximated approach was proposed by Park and Pande (2007) to circumvent this difficulty. Here we present a detailed study about this procedure by comparing its performance with exact (free-energy) weights and other methods, its dependence on the total replica number R and on the temperature set. The ideas above are analyzed in four distinct lattice models presenting strong first-order phase transitions, hence constituting ideal examples in which the performance of algorithm is fundamental. In all cases, our results reveal that approximated weights work properly in the regime of larger R's. On the other hand, for sufficiently small R its performance is reduced and the systems do not cross properly the free-energy barriers. Finally, for estimating reliable temperature sets, we consider a simple protocol proposed by Valentim et al. (2014).

1. Introduction

Although Monte Carlo method has become probably the most common tool for studying phase transitions and critical phenomena, in practice its usage is not so simple, whenever standard algorithms (e.g. Metropolis) are used. Despite the simplicity and generality, they lead to difficulties close to the emergence of phase transitions. For instance, alternative procedures are typically required, specially in the case of systems with microscopic configurations separated by valleys and hills in the free-energy landscape [1–4]. Cluster algorithms [5,6], multicanonical [7], Wang–Landau [8] and tempering methods are some examples of proposals to overcome these difficulties. In particular, parallel tempering (PT) [9] and simulated tempering (ST) [10] enhanced sampling methods have drawn attention due to their generality and simplicity when compared with the previous examples. Their basic idea consists of using configurations from high temperatures for systems at low temperatures, allowing in principle the dynamics to escape from metastable states and providing an appropriate visit of the configuration space. In particular, distinct aspects of tempering methods have been explored in the last years, aiming at better understanding of efficiency and pertinence. For instance, the role of temperature sets for the PT case was investigated in Refs. [11–14], whilst the importance of non-adjacent exchanges was taken into account in Refs. [14–18]. In addition the efficiency and comparison between tempering methods were considered in Refs. [19–21].

Focusing our attention in the ST we face one of its main difficulties, namely the evaluation of the free-energy weights, required for a uniform sampling to all temperatures. Despite the development of alternative techniques, their applicability for more complex systems still poses a hardship. In some cases [19,22], the accumulation of histograms (of a given quantity) and previous simulations are necessary to calculate (or to estimate) the input parameters that guarantee a sufficient number of visits to all temperatures. In such cases, the weights are set arbitrarily but a knowledge of the partition function Z_i at each temperature is required and a flattening histogram based on a random walk in the parameter (temperature or energy) space is used to obtain a satisfactory estimation of Z_i. In Refs. [23,24], the partition function is exactly valued through numerical simulations, taking into account its relationship with the largest eigenvalue $\lambda^{(0)}$ of the transfer matrix

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$\mathcal{T}$. Although the evaluation of $\lambda^{(0)}$ is possible for lattice-gas systems, its extension for more complex cases (e.g. off-lattice systems) is not straightforward. In contrast to previous "exact" approaches, Park and Pande [25] proposed an approximated tool of estimating weights, based on the average system energy. Since the mean energy is easily obtained for any system (including lattice and off-lattice models), it constitutes a considerable simplification over the free-energy case. Nevertheless, there are some fundamental points that need to be understood in order to make it a promptly useful method. The first one is how this procedure compares itself with using free-energy weights? The second one is under what conditions does it provide equivalent results to those obtained from free-energy weights? An additional point is if it is possible to obtain proper temperature set that yields precise results under lower computational cost. To answer the aforementioned points, we have analyzed, under the ST with approximated weights, four distinct lattice models, namely, Blume–Capel (BC) and Blume–Emery–Griffiths (BEG) [26], Bell–Lavis (BL) [27,28] and associating lattice gas (ALG) water models [29,30]. The former two are interesting tests, due to the existence of very precise results available from cluster algorithms [31], Wang–Landau [32], PT and ST with free-energy weights [14,18,20,33]. Therefore, they constitute relevant benchmarks for our purposes. The BL and ALG are also important examples, taking into account their more complex phase diagrams, including liquid phases with distinct structures, regions of unusual behaviors (density and diffusion anomaly lines) and also dynamic transitions [28,34]. In the case of ALG, an extra advantage arises, due to the existence of two phase coexisting lines, between gas and liquid phases. Hence, the ALG works as a double checking of reliability of our proposals. For instance, we focus on the regime of low temperatures, in which strong first-order phase transitions separate coexisting phases. Recently a general approach for discontinuous transitions has been proposed [35,36], in which thermodynamic quantities are described by a general function, allowing to achieve all relevant information by studying rather small system sizes for some control parameters. Thus, its combination with a proper usage of ST can provide us a powerful approach to deal with discontinuous transitions with rather low computational cost.

Henceforth, the analysis of all cases will show that the approximated weights work properly (and hence lead to correct results) in the regime of large replica numbers R for an appropriate choice of temperature sets [33]. On the other hand, for sufficiently small R its performance is strongly reduced and the system does not visit properly the distinct coexisting regions. Finally we extend for the approximated weights, a simple protocol for obtaining proper temperature sets initially proposed for the free-energy weights [33].

2. Simulated tempering and approximated weights

The basic idea of the ST concerns with the fact that the system temperature T can assume different values between the extreme values T_1 and T_R, where R is the replica number. The MC simulation is defined as follows: In the first part, starting at a given temperature T_i within the set $\mathcal{T}_R \equiv \{T_1, \ldots, T_R\}$ (in all cases we started from T_R), a given site of the lattice is randomly chosen and its variable is changed (among all possibilities) according to the Metropolis prescription $\min\{1, \exp(\beta_i \Delta\mathcal{H})\}$, where $\Delta\mathcal{H}(\sigma)$ denotes the energy difference between the "new" and "old" configurations and $\beta_i = 1/k_B T_i$. After repeating above dynamics a proper number of realizations (here L^2 random choices are considered) in the second part the temperature exchange ($T_i \to T_j$) occurs with the following probability

$$p_{i\to j} = \min\{1,\ \exp[(\beta_i - \beta_j)\mathcal{H}(\sigma) + (g_j - g_i)]\}, \tag{1}$$

where g_i is the weight associated with the temperature T_i and $\mathcal{H}(\sigma)$ is the system Hamiltonian. For a uniform sampling, the weights should be proportional to the free-energy f_i given by $g_i = \beta_i f_i$ [25]. Since the evaluation of f is not an easy task, alternative calculations of weights have been proposed [19,22–24]. The simplest proposal [25] estimates the g's according to the following approximated formula

$$g_j - g_i \approx (\beta_j - \beta_i)(U_j + U_i)/2, \tag{2}$$

with $U_i = \langle \mathcal{H}_i \rangle$ $(i = 1, 2, \ldots, R)$ denoting the average system energy at T_i. Thus, from Eq. (2) the weights are estimated from simple and direct standard numerical simulations. Here we give a further step by analyzing them by inspecting two crucial points: their dependence on the replica number R and on the set of temperatures $\mathcal{T}_R$. In order to scrutinize them, we compare numerical results at the phase coexistence points for distinct R's, with temperature schedules estimated as proposed in Ref. [33] and described as follows: starting from a fixed T_1 we choose the next $R-1$ temperatures $T_2 < T_3 < \cdots < T_R$ in such a way that the resulting exchange frequencies $f_{i+1,i}$ between any two successive temperatures T_i and T_{i+1} are all equal to some value specified $f_{i+1,i} = f$. We define $f_{i+1,i}$ as the ratio of the number of exchanges between T_i and T_{i+1} to the total Monte Carlo steps N_{MC}. Note that from this recipe the highest temperature T_R becomes automatically obtained. The efficiency of such achieved set $\mathcal{T}_R$ is verified by means of standard tests, where in the case of first-order transitions, the tunneling between the coexisting phases and convergence to the steady state starting from a non-typical initial configuration constitute proper efficiency measures. More specifically, the existence of full trapping in a given phase or even temperature changes that do not allow the system to visit properly the coexisting phases will imply in thermodynamic averages marked by no changes or abrupt variations (see Fig. 2 for $f = 0.37$ and $f = 0.02$, respectively). Such points can be understood by recalling the ideas from Refs. [35,36], when the system close to the phase coexistence have typical thermodynamic quantities, like energy and order parameter, well described by the following general expression

$$W(y) \approx \left(b_1 + \sum_{n=2}^{\mathcal{N}} b_n \exp[-a_n y]\right) \Big/ \left(1 + \sum_{n=2}^{\mathcal{N}} c_n \exp[-a_n y]\right), \tag{3}$$

where for $\mathcal{N}$ coexisting phases, y denotes the "distance" to the coexistence point ξ^* given by $y = \xi - \xi^*$. The coefficients c_n's and b_n's are related to derivatives of the free energies f_n of each phase n with respect to parameter ξ reading $\partial f_n/\partial\xi$ [36]. In the case of two phase coexistence ($\mathcal{N} = 2$) Eq. (3) acquires the following way $W(y) = (b_1 + b_2 \exp[-a_2 y])/(1 + c_2 \exp[-a_2 y])$ and hence only four parameters are necessary to determine the whole function. In other words, according to Eq. (3), numerical simulations (of a given system) for known L and control parameter sets $\xi = \xi_0$ (like chemical potential and temperature) will provide a well defined value for thermodynamic quantities $W_0^* = W(L, y_0)$, where $y_0 = \xi_0 - \xi^*$. Note that at the phase coexistence point $y = 0$, the quantity W reads

$$W_0 = \frac{b_1 + \sum_{n=2}^{\mathcal{N}} b_n}{1 + \sum_{n=2}^{\mathcal{N}} c_n} \tag{4}$$

for all L's. Hence, different curves of W should cross at the coexistence point. However, as W_0 and W_0^* are verified only for dynamics that visit properly the distinct phases (e.g. one flip algorithms lead to strong hysteresis at low T's and results do not obey Eq. (3)). In the case of tempering methods, the achievement of results not following Eq. (3) indicates that $\mathcal{T}_R$ is not proper. Typically, low T_i's (including the extreme T_R) provide high temperature exchanges,