Nonflat Histogram Techniques for Spin Glasses

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(Dated: November 18, 2020)

We study the bimodal Edwards-Anderson spin glass comparing established methods, namely the multicanonical method, the $1/k$-ensemble and parallel tempering, to an approach where the ensemble is modified by simulating power-law-shaped histograms in energy instead of flat histograms as in the standard multicanonical case. We show that by this modification a significant speed-up in terms of mean round-trip times can be achieved for all lattice sizes taken into consideration.

I. INTRODUCTION

Simulations of systems with rugged free-energy landscape [1] suffer from massive slowing down of the dynamics in the low-temperature phase. This problem encountered in many physical systems, e.g., folding polymers or spin glasses, renders the investigation of the thermodynamical properties of such systems in the low-temperature phase a very challenging task.

The Metropolis algorithm [2] is designed to sample configurations according to their statistical weight in the canonical ensemble. At low temperatures it fails dramatically for systems with rugged free-energy landscape because of the effectively broken ergodicity. The simulations get stuck in local minima (metastable states) and the thermal energy is not sufficient to overcome the huge free-energy barriers. There have been a wide range of algorithmic developments tackling this problem that can all be subsumed in the term of broad-energy ensembles.

One commonly employed method is the Parallel Tempering (PT) [3–5] method where Metropolis simulations of copies of the system (replicas) at different temperatures are performed. After certain time intervals exchanges of the replicas between the different temperatures are attempted. This procedure enables the replicas at low temperature to fully explore deep free-energy valleys and at high temperature to travel freely through the phase space and thus to decorrelate. Thereby, the different replicas can explore the rugged structure of the free-energy landscape much more efficiently than in a simple Metropolis simulation. Using this method at temperatures close to the transition, studies of spin-glass systems of sizes up to $40^3$ spins have been reported [6, 7]. For ground-state searches systems of about $10^4$ are feasible [8]. The great advantage of PT is its simplicity: the algorithm only needs a suitable temperature set and exhibits good performance which makes it probably the most employed method in the investigation of systems with rugged free-energy landscape.

Another recent development is the Population Annealing Monte Carlo [9–13] method which proceeds similarly to Simulated Annealing [14] as the system is gradually cooled down according to an annealing schedule. The annealing is performed on a big population of replicas and by introducing intermediate resampling of the population of replicas after lowering the temperature the simulation is kept at thermal equilibrium. This permits the evaluation of thermodynamic observables in contrast to simple Simulated Annealing. Despite the attempts of optimizing the method for spin glasses [10, 12, 15] it is not able to outperform PT. Its optimization, however, remains more cumbersome due to the additional complexity. The main advantage of this algorithm is its suitability for massively parallel implementation. For disordered systems, however, this advantage does not come into play, because the necessity of simulating many different disorder realizations allows the efficient use of parallel computing for any method.

The Multicanonical (MUCA) method [16–18] is another well-established algorithm designed for the simulation of systems with first-order phase transitions which performs well in the simulation of systems with rugged free-energy landscape, too. It has already been applied to spin glasses in Refs. [19, 20]. In this method the simulation is set up to visit all possible energies with the same probability yielding a flat histogram in energy. However, it has been noted by different researchers that this ensemble is not optimal. One suggested improvement is the $1/k$-ensemble by Hesselbo and Stinchcombe [21], where the sampling distribution is the inverse of the integrated estimator of the local diffusivity in order to maximize the number of performed round trips in energy. The method is among others applied to the ferromagnetic Ising model for which it improves the scaling behavior of the round-trip times in energy. The improved performance for the models considered in that work and the nature of the algorithm of automatically identifying the bottlenecks of the simulation and concentrating the simulation effort on this region suggest that the round-trip times of the simulations should diminish independently of the underlying system. However, in our implementation, in the case of

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the three-dimensional (3D) bimodal Edwards-Anderson (EA) spin glass [23], the round-trip times did not systematically improve with this method. Instead the simulation got stuck for some of the considered samples, rendering a comparison to the other methods impossible.

In this work we present a different approach: we prescribe parametric profiles for the histograms of the simulation and adjust the simulation weights accordingly. As for the three previous MUCA variants, it requires the knowledge of the underlying density of states, but it is much more flexible. The profiles are all chosen to be shifted power laws having two free parameters.

As an example we consider the 3D bimodal EA spin glass. This is one of the simplest models exhibiting a rugged free-energy landscape and is also interesting from the point of view of an optimization problem where finding ground states of hard disorder realizations is NP-hard [24]. Despite the exponential growth of the computational resources fundamental questions regarding the nature of the spin-glass phase still remain. For the progress in understanding the open questions the development of new methods and an improvement of the existing methods is crucial.

The rest of the paper is organized as follows. In Sec. II the spin-glass model and the simulation methods are explained. The direct comparison of the round-trip times of the individual methods is performed in Sec. III. The framework of extreme-value statistics is introduced in Sec. IV. In Sec. V benchmarks for the global comparison are discussed and the different methods are compared in terms of those benchmarks. The results are summarized in Sec. VI.

II. MODEL AND EMPLOYED METHODS

We take into consideration the 3D bimodal EA model whose Hamiltonian takes the form

$$ H = -\sum_{<i,j>} J_{ij} S_i S_j, \quad (1) $$

where the bonds $J_{ij}$ and the spins $S_i$ can take values $\pm 1$. The sum runs over all neighboring spins in the simple-cubic lattice with periodic boundary conditions.

Due to the disordered nature of spin glasses the study has to take into account a sufficiently large set of disorder realizations on which the averaged quantities can be computed. In this case one disorder realization consists of a set of $3V$ couplings $J_{ij}$ which are either positive or negative unity with a probability of 50%, where $V = L^3$ is number of spins in a lattice of linear lattice size $L$. The disorder realizations are generated prior to the simulation and then kept fixed for all times (quenched disorder). As an adequate set of disorder realizations 4000 samples with $L = 3$ and $L = 4$ are generated and 5000, 6000, and 4000 samples of size $L = 5, 6, \text{ and } 8$, respectively.

The method which we adapted is the well-established MUCA method [17] employing a generalized Metropolis criterion with an energy dependent weight function

$$ P_{\text{acc}} = \min \left( 1, \frac{W(E_{\text{new}})}{W(E_{\text{old}})} \right), \quad (2) $$

where the weight function is proportional to the inverse of the density of states $\Omega(E)$,

$$ W(E) \propto \Omega^{-1}(E). \quad (3) $$

For the MUCA simulations $\Omega(E)$ has to be sufficiently well-known a priori for each disorder realization. An estimator for it can, for instance, be obtained by means of the Wang-Landau algorithm [25] or, as in this work, by other iterative procedures which are explained, e.g., in Ref. [26]. This ensemble produces histograms which are flat in energy and is, therefore, often also referred to as “flat histogram method”.

A straightforward generalization of the flat histogram method are the nonflat histogram methods. If the simulation weights for the flat MUCA method are multiplied with the desired energy dependent shape (or profile) function $P_{\text{SH}}(E)$

$$ W(E) \propto \Omega^{-1}(E) P_{\text{SH}}(E), \quad (4) $$

the resulting histograms will be shaped according to $P_{\text{SH}}(E)$. In this work all the profiles are shifted power laws of the form

$$ P_{\text{SH}}(E, \Delta E, \alpha) = \left( \frac{E}{\Delta E - E_g} + 1 \right)^\alpha, \quad (5) $$

where the exponent $\alpha < 0$ and $\Delta E > 0$ is the position of the pole relative to the ground-state energy $E_g$ of the respective spin-glass realization. In this parametrization the power laws are normalized to unity at $E = 0$.

In Fig. 1 the recorded histograms of the different methods are displayed on a logarithmic $y$-scale for one disorder realization with $L = 8$. In contrast to flat MUCA all

![Figure 1](image-url)
methods have in common that the distribution of sampled states grows towards the ground-state energy. The recorded histogram of nonflat MUCA matches perfectly the imposed profile and its histogram in the ground-state region is similar to that of PT. We are convinced that this feature which among the existing methods is strongest for PT enhances the ability of sampling the low-energy region and especially the ability of finding low-energy states of investigated systems. There are different possible choices of functional forms which enhance the sampling of the low-energy region and even stepwise defined function could be employed and might even yield better results. We chose a power law because the two involved parameters allow for a good adaptation but the tuning of the parameters in the two-dimensional parameter space remains feasible.

For the above parametrization we found a fixed parameter set namely $\alpha = -3.6$ and $\Delta E = 96$ which independently of the lattice size yielded the shortest mean round-trip times, among the considered profiles. Subsequently we will refer to the nonflat MUCA setting with the power-law shape belonging to this parameter set just as power-law (PL) setting or nonflat MUCA method. While the overall best results are obtained with this parameter set, we want to point out that an improvement compared to flat MUCA was visible for each of the considered parameter sets. The parametrization with a fixed offset from the ground-state energy yields different relative distributions depending on the ground-state energy encountered in the respective disorder realization. The value of the profile function at the ground-state energy is given by

$$P_{SH}(E_g, \Delta E, \alpha) = \left(\frac{1}{1 + \frac{E_g}{\Delta E}}\right)^\alpha. \quad (6)$$

The sampling at the ground-state energy compared to zero energy is thus enhanced by a factor of $\approx 13$ for a disorder realization with $L = 4$ and a typical ground-state energy of $\approx -100$. For a sample with $L = 8$ and typical ground-state energy of $\approx -900$ instead it is enhanced by a factor of $\approx 4500$. Due to this feature this parametrization of the profile function does not require any adjustments of the parameters in the system sizes which we considered. Presumably such a profile will also yield good results for larger systems, although we cannot be certain.

Next the $1/k$-ensemble [21] is considered which is defined by setting the simulation weights equal to the inverse of the integrated density of states up to the energy of the respective bin

$$W_{1/k}(E) \propto 1/k = \left(\int_{E_g}^{E} dE' \Omega(E')\right)^{-1}. \quad (7)$$

Here, a first-order Taylor expansion of $\ln \Omega$ at $E$ leads to $W(E) \approx W_{1/k}(E)$ if $P_{SH}(E) = d \ln \Omega(E')/dE'|_{E'=E}$. This prescription again relies on the knowledge of the density of states. The authors of Ref. [21] stress its robust ergodicity and apply it to spin glasses and the traveling salesman problem [21].

Since for the above mentioned methods the density of states is the only needed input it was determined only once to high accuracy employing the iterative procedure adapted from Ref. [22] but with power-law shaped distributions in energy. In this case, and generally when the ground-state energy of the system is not known, a priori the profile function has to be adapted whenever a lower energy is found.

Lastly, the PT method being probably the most employed algorithm for spin-glass simulations, is included in the comparison. The ensemble in this case is defined by a set of $M$ temperatures $\{T_i, i = 1, ..., M\}$. For each temperature $T_i$ a Metropolis simulation of a copy of the system (replica) is performed. The temperatures of the replicas $i$ and $j$ are allowed to exchange configuration according to

$$P_{ex}^{ij} = \min \left(1, e^{(\frac{1}{k_B T_i} - \frac{1}{k_B T_j})(E_j - E_i)}\right), \quad (8)$$

where $E_i$ and $E_j$ are the energies of replica $i$ and $j$ and $k_B = 1$. This prescription allows for fast decorrelation when a replica travels to high temperature and the exploration of the local minima at low temperatures. Among the vast choice of different PT protocols available [28] we opted for the constant exchange rate protocol with acceptance rates between $40\%$ and $60\%$ [29]. For all simulations the maximal temperature was chosen to be well above the critical temperature, $T_{max} > 3 > T_c \approx 1$. The exchange rates were imposed on each individual disorder realization in an initial equilibration run during which the temperatures were modified accordingly. The number of replicas was set to $M = 7, 7, 12, 14$, and $20$ for $L = 3, 4, 5, 6$, and $8$, respectively. We note that the choice of the temperature set is crucial for the PT algorithm and also provides the possibility of optimizations as for example in Ref. [30]. However, in this work we rather limit ourselves to a well established protocol for PT focusing on the optimization of the nonflat histogram technique.

### III. COMPARISON OF THE ROUND-TRIP TIMES

The observable taken into account for this study is the round-trip time. For all methods except PT and each disorder realization it is defined as the time needed by the simulation to travel from the highest energy ($E \approx 0$) to the ground-state energy and back. For PT, instead, the round trip is measured between the ground-state energy and an energy typical for a canonical ensemble with a temperature well above the freezing point of the disorder realization [31][32]. This time can be taken as an upper bound of the autocorrelation time of the energy of the respective disorder realization at the ground state. We want to stress that the energies we refer to as ground-state energies are the lowest encountered energies and
may not be the true ground states. However, the round-trip times were always measured performing at least 100 round trips for each individual sample and method so that several hundred round trips have been performed on each disorder realization. In case lower energies were measured during this process the disorder realization was requeued and simulated again until the desired number of round trips was achieved. This procedure renders the discovery of the true ground state very probable. After at least 100 round trips the relative statistical error in the round-trip time $\tau_i$ is of the order of $\Delta\tau_i/\tau_i \approx 0.1$.

The first property we want to look at is the dependence of the round-trip times for the individual disorder realizations on the employed method. The scatter plots in Fig. 2 show the round-trip times of the same disorder realization for two different methods for all the simulated disorder realizations of size $L = 4$ and $L = 8$ on a log-log scale. The strong correlation of the round-trip times for each single disorder realization should be noted, indicating that the hardness of the underlying optimization problem is primarily a characteristic of the disorder realization and mostly independent of the employed method. This fact allows us to categorize the disorder realizations and speak of easy and hard instances. Comparing the round-trip times $\tau_i$ for the flat MUCA method and the parallel tempering method (left panels) for both lattice sizes $L = 4$ and $L = 8$, the $\tau_i$ are systematically lower for PT, indicating its superior performance for the whole classes of the bimodal EA spin glasses of the respective lattice sizes.

When comparing the performance of the nonflat histogram method to the flat MUCA method (central panels) the surrounding area of the scattered round-trip times shows a bending, i.e., for $L = 4$ the flat histogram method displays only slightly higher round trip times for the easy disorder realizations. With increasing hardness the round-trip times for the flat histogram method grow faster than for the PL setting. This effect gets enhanced with a further increase of the lattice size (see lower panel) where for the case of $L = 8$ the round-trip times of the easiest samples for the flat MUCA method are similar to those for PL. However, as will become apparent in the next section, the hard samples contribute most to the mean round-trip time so that even a slightly weaker performance for the easier samples would hardly contribute to the total computation time.

The right panels show the comparison of PL to PT. For $L = 4$ PT outperforms the nonflat histogram method for the easy disorder realizations, while for the hard ones PL displays shorter round-trip times. For $L = 8$ a large
fraction of the disorder realizations is characterized by shorter round-trip times for PT, but the tail of the distribution describing the hard samples exhibits shorter round-trip times for PL.

IV. ROUND-TRIP TIME DISTRIBUTIONS

In order to quantify the observations of the previous section the distributions of the round-trip times can be examined. Round trips in energy include the visit of the ground state of the respective disorder realization which is an extreme event. Their statistics must thus be described in the framework of extreme-value statistics. One of the main results in this field is given by the Fisher-Tippet-Gnedenko theorem [33] which characterizes the type of distributions which extreme-value distributions can converge to. The round-trip time distributions of the bimodal EA spin glass all seem to converge to Fréchet distributions independently of the method and the system size. This has already been suggested in Ref. [34] for the round-trip time distributions of the 3D EA model employing the flat histogram ensemble.

One parametrization of the cumulative distribution function (CDF) of the Fréchet distribution is given by

$$F(\tau) = \exp \left[-\left(1 + \frac{\tau - \mu}{\beta} \right)^{-1/\xi}\right], \quad (9)$$

with $\tau \in [\mu - \beta/\xi, \infty)$. The location of the distribution along the $\tau$-axis is determined by $\mu$, $\beta$ is the scale parameter, and the shape parameter $\xi$ describes the decay of the tail of the distribution, i.e., the occurrence of rare events. The CDF is the integrated form of the probability density function (PDF) $f(\tau)$. The round-trip time distributions are thus all defined by sets of parameters $\mu, \beta, \xi$ which are determined by fitting the CDF to the recorded round-trip times.

The measured round-trip times and the respectively best fitting Fréchet distribution for lattice sizes $L = 4$ and $L = 8$ are plotted in Fig. 3. The points represent the measured data and the solid lines are the best fitting Fréchet distributions. The varying performance of the methods in dependence on the difficulty of the disorder realizations which became visible in the last section, also reflects in the distribution of the round-trip times. For both lattice sizes the CDF belonging to the flat MUCA method is lower for all $\tau$ than the one belonging to PT. The maximum increase which corresponds to the bulk of the distribution is shifted to higher $\tau$ for MUCA as compared to PT.

Comparing PT instead to the PL setting yields a different picture: the cumulative distribution functions for lattice size $L = 4$ cross at $F(\tau) \approx 1/3$, corresponding to a round-trip time $\tau \approx 2 \times 10^2$. This means that for the PT algorithm the easiest one third of all samples have smaller round-trip times than the easiest third for the PL method, while PL is faster for the harder two thirds. For $L = 8$ the PL round-trip times are larger for the easier half of the samples and smaller for the harder half. The round-trip times for the hard disorder realizations

FIG. 3. Round-trip time distributions (symbols) and best fitting cumulative distribution functions (lines) for the different methods and lattice size $L = 4$ (a) and $L = 8$ (b). The inset of the left panel shows the PDF form of the distribution.

FIG. 4. The figure shows the shape parameter of the best fitting Fréchet distribution in dependence of the lattice size for the different employed simulation methods. The dotted line indicates the threshold value from which on the distribution mean diverges.
A. Finding a Benchmark

In principle the real performance could be determined by measuring the round-trip time of every possible disorder realization. This procedure is discarded due to the enormous number of possible disorder realizations. Instead we generate a subset of all possible disorder realizations and from those we try to infer the expected mean round-trip time of all the disorder realizations belonging to the same problem class, by means of the population mean $\tau_{\text{pop}}$. This is a standard approach in all Monte Carlo studies and the law of large numbers assures its convergence for all random variables from distributions with well defined mean. However, this prerequisite is not fulfilled for all of the round-time distributions encountered in this work.

The expected mean round-trip time resulting from the underlying probability density could be estimated by the distribution mean

$$\langle \tau \rangle = \int_{\mu - \beta/\xi}^{\infty} d\tau f(\tau).$$  \hspace{1cm} (10)

This integral can be computed analytically, yielding

$$\langle \tau \rangle = \left\{ \begin{array}{ll}
\mu + \frac{\beta}{\xi} \Gamma(1 - \xi) - 1 & \text{for } \xi < 1 \\
\infty & \text{otherwise}
\end{array} \right. ,$$  \hspace{1cm} (11)

with $\Gamma(x)$ being the gamma function. The distribution mean is, therefore, only defined as long as the shape parameter $\xi$ is smaller than one. To illustrate this difficulty one can consider the running mean which is defined as the population mean over the first $n$ generated disorder realizations keeping them in a fixed order,

$$\tau(n) = \frac{1}{n} \sum_{i=1}^{n} \tau_i ,$$  \hspace{1cm} (12)

implying $\tau_{\text{pop}} = \tau(N)$, where $N$ is the number of all simulated disorder realizations.

In Fig. 5 the running mean for the flat MUCA method and different system sizes is plotted together with the respective distribution mean, if it is defined. For $L = 4$ ($\xi \ll 1$) the running mean quickly converges to the distribution mean indicated by the dotted line. For $L = 6$ ($\xi \approx 1$) the jumps due to rare events in the tail of the distribution become more pronounced. The running mean is still expected to approach the distribution mean for a finite number of disorder realizations. For the 6000 samples considered in our work this is still not the case. For $L = 8$ ($\xi > 1$) the distribution mean is not defined. In the picture of the running mean, jumps represent round-trip times in the tail of the distribution. In the case of $\xi > 1$ those jumps $\tau_i/n$ in the running mean are clearly visible in Fig. 5 and will lead to a divergence of the population mean the more disorder realizations are taken into account and hence the more rigorously the tail of the distribution is explored. This illustrates that the population mean as a measure for the performance of the different methods must be taken with a grain of salt.

In order to retain the characteristics of the underlying round-trip time distribution into the estimator of the performance of the different methods the distribution mean up to a certain quantile can instead be taken into account.
The quantile function is the inverse of the CDF, 
\[ Q(p) = F^{-1}(p) = \mu + \frac{\beta}{\xi} \left( (-\ln p)^{-\xi} - 1 \right), \quad p \in (0, 1), \]
yielding the round-trip time \( \tau_p = Q(p) \) at which a certain fraction \( p \) of the distribution is accumulated. For each \( \epsilon < 1 \) we define the quantile mean \( \langle \tau \rangle_{\epsilon} \) disregarding a fraction \( \epsilon \) of the tail of the distribution as the integral
\[ \langle \tau \rangle_{\epsilon} = \int_{\mu - \beta / \xi}^{Q(1-\epsilon)} d\tau f(\tau). \]

The integral is evaluated with the parameters of the best fitting distributions to the measured round-trip times, see Fig. 3. This enables a well-defined extrapolation beyond the measured round-trip times of the simulated disorder realizations of the underlying study and thus a comparison of the different methods beyond the mere population mean, which may be strongly dependent on the set of disorder realizations taken into account for the study.

### B. Comparison of the Different Methods

Finally, for the comparison of the mean round-trip times only the population mean \( \tau_{\text{pop}} \) and the quantile mean \( \langle \tau \rangle_{\epsilon=10^{-4}} \) neglecting a fraction \( \epsilon = 10^{-4} \) of the tail of the distribution are taken into account as the distribution mean for the parallel tempering method is already ill-defined for \( L = 6 \).

The two definitions are evaluated for all simulated lattice sizes and plotted in Fig. 3. Both definitions of the mean grow exponentially up to linear system size \( L = 6 \) until which the mean is defined, while for \( L > 6 \), where the distribution means diverge, they seem to be growing faster than exponentially. We have also looked at the scaling of the more commonly used quantiles including the median \cite{38, 39}, which are derived directly from the \( \tau \)-values without the intermediate step of fitting to a statistical model. These quantiles behave similarly to the quantile means \cite{14} being, however, less stable for small \( \epsilon \).

For the direct comparison of PL with the existing methods we introduce the relative performance \( r \) which we define as the fraction of the mean of the respective method and the one of PL. In Table I, the relative performance for all different system sizes is listed. The errors in \( r \) are estimated using the Jackknife resampling technique. It consists in generating a set of ratios \( \{ r_i \} \), where for the calculation of each \( r_i \) only a subset of all disorder realizations is taken. The error in \( r \) is derived from the variance of the so generated Jackknife sample.

The speedup of PL compared to flat MUCA increases with system size, reaching a factor of more than 10 for \( L = 8 \) for both definitions of the mean, while compared to the 1/k ensemble the speedup for the biggest system size is still a factor of \( r \approx 7 - 9 \). Compared to PT the speedup is less pronounced and not steadily growing with system size, reaching a factor of \( r \approx 2 - 3 \) for our largest system sizes.

### Table I. Ratios of the population mean \( \tau_{\text{pop}} \) and the quantile mean \( \langle \tau \rangle_{\epsilon=10^{-4}} \) of the round-trip times for flat MUCA, the 1/k-ensemble, and parallel tempering with respect to the same quantities for the power-law MUCA method.

| \( L \) | \( \tau_{\text{pop}} \) | \( r_{\epsilon=10^{-4}} \) | \( \tau_{\text{pop}} \) | \( r_{\epsilon=10^{-4}} \) | \( \tau_{\text{pop}} \) | \( r_{\epsilon=10^{-4}} \) |
|---|---|---|---|---|---|---|
| 3 | 1.160(2) | 1.174(3) | 1.0146(6) | 1.0193(9) | 1.637(4) | 1.640(5) |
| 4 | 1.622(8) | 1.68(2) | 1.288(5) | 1.328(10) | 1.175(6) | 1.25(2) |
| 5 | 2.28(5) | 2.44(6) | 1.63(3) | 1.75(4) | 1.136(3) | 1.185(8) |
| 6 | 3.8(2) | 3.9(2) | 2.59(9) | 2.6(2) | 2.8(2) | 3.4(3) |
| 7 | 10.5(2) | 14.2(6) | 6.9(3) | 9.4(4) | 2.1(2) | 2.62(7) |
VI. CONCLUSION

Setting up multicanonical simulations such that the
outcoming histograms are shaped according to power
laws instead of being flat is trivially achievable. Nev-
evertheless this simple approach enables us to gather sig-
nificantly more independent statistics at the ground-state
energy, which is important because the thermodynamic
contributions of the ground state of spin glasses are be-
lieved to be significant. It is likely that similar techniques
will also improve the sampling of the ground state of
other systems with complex free-energy landscape such
as polymers and in particular proteins, for which the im-
portance of the native state is well known.

While PT has been the most employed method in the
simulation of spin glasses probably also due to its good
ability to investigate the ground-state region, we were
able to show that the power-law setting considerably im-
proves the performance of multicanonical simulations in
this respect, rendering them at least comparable to PT.

The overall gain in performance grows with increasing
lattice size and reaches a factor of up to $10 - 15$ in com-
parison to flat MUCA and still a factor of up to $2 - 3$
compared to PT. In terms of round-trip time distribu-
tions the heaviness of the tails is reduced by its superior
ability to deal with the hard disorder realizations.

This improved ability of the here proposed power-law
MUCA method of finding ground states for the hard in-
stances implies its usefulness in the application to gen-
eral optimization problems. This is particularly use-
ful because many other optimization problems can be
rephrased in terms of spin-glass Hamiltonians and thus
solved employing the same methodology.

ACKNOWLEDGEMENT

This project was funded by the Deutsche Forschungs-
gemeinschaft (DFG, German Research Foundation) un-
der project No. 189853844 – SFB/TRR 102 (project
B04). It was further supported by the Deutsch-
Französische Hochschule (DFH-UFA) through the Doc-
toral College “L4” under Grant No. CDFA-02-07.

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