BRIEF REVIEW OF MULTICANONICAL SIMULATIONS

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Recent progress of simulations with non-canonical weights is summarized.

1 Introduction

One of the questions which ought to be addressed before performing a large scale computer simulation is “What are suitable weight factors for the problem at hand?” It has been expert wisdom for quite a while that Monte Carlo (MC) simulations with a-priori unknown weight factors are feasible and deserve to be considered.1 With focus on narrow classes of applications, this idea was occasionally re-discovered, for instance.2 But it needed the work of Ref.3,4 to become a more widely accepted idea in Statistical Physics as well as in Lattice Gauge Theory.

The next section introduces systems with supercritical slowing down. Section 3 reviews the multicanonical (MUCA) approach and briefly sketches related methods. Applications to first-order phase transitions are summarized in section 4 and those to systems with conflicting constraints in section 5, before some conclusions are drawn in section 6. Some interesting topics, like the dynamical-parameter method in U(1) gauge theory, had to be omitted because of space limitations. For a MUCA calculation of constraint effective potentials see Neuhaus in these proceedings.

2 Supercritical Slowing Down

The terminology “supercritical slowing down” is used to characterize canonical MC simulations which slow down exponentially fast with increasing system size. It is useful to distinguish static and dynamic reasons for the slowing
down. In the former case desired configurations have an exponentially small weight, whereas in the latter case their weight may still be large, but the dynamic process of reaching them deteriorates.

**Static Examples:**

- Magnetic field driven first-order phase transitions: Configurations with zero (or small) magnetic fields are exponentially suppressed at low temperatures and they exhibit domain walls.

- Temperature driven first-order phase transitions: Configurations with domain walls are exponentially suppressed.

**Dynamic Examples:**

- Low temperature transitions between magnetic states (for instance the up-down states of the Ising model below the Curie temperature, ...).

- Transition between low temperature states in systems with conflicting constraints: Spin glasses, the traveling salesman problem, ...

3 Multicanonical and Related Methods

These methods try to overcome supercritical slowing down by sampling with *unconventional weights*.

Canonical MC simulations perform importance sampling with respect to the Boltzmann weight

\[ w_B = e^{-\beta E} \]

Using reweighting, expectation values in a vicinity (\( \to 0 \) for \( V \to \infty \)) of the temperature \( T = 1/\beta \) are obtained.

**Multicanonical** refers to simulations which obtain expectation values for a temperature range, which stays finite in the limit \( V \to \infty \).

Similarly, **multimagnetical** refers to simulations which give results for a certain range of the magnetic field, etc. ... . The cluster variant \(^7\) is called **multibondic**.

3.1 *How to get MUCA results?*

The aim is to sample a broad energy density, like the uniform

\[ P(E) = \text{const. for } E_{\min} < E < E_{\max} \]
where $e_{\text{min}} = E_{\text{min}}/V$ and $e_{\text{max}} = E_{\text{max}}/V$ may be kept constant. The uniform density is obtained by sampling, for $E_{\text{min}} < E < E_{\text{max}}$, with the weight factor

$$w(E) = 1/n(E)$$

where $n(E)$ is the spectral density. As $n(E)$ is a-priori unknown, some preliminary or iterative estimate of $n(E)$ has to be part of the approach. For attempts to optimize the weight factors see $^8$.

### 3.2 Weight factors and temperature

Let us re-write the weight factor as

$$w(E) = e^{-S(E)} = e^{-\beta(E)E + \alpha(E)}$$

where $S(E)$ is the microcanonical entropy. Then, the temperature follows from

$$T(E) = 1/\beta(E) \quad \text{and} \quad \beta(E) = \frac{\partial S(E)}{\partial E}$$

Further, the function $\alpha(E)$ is determined up to an additive constant.

*Example with discrete energy:*

$$\beta(E) = \frac{|S(E + \epsilon) - S(E)|}{\epsilon} \quad (\epsilon \text{ smallest energy step})$$

The identity $S(E) = \beta(E)E - \alpha(E)$ implies

$$S(E) - S(E - \epsilon) = \beta(E)E - \beta(E - \epsilon)(E - \epsilon) - \alpha(E) + \alpha(E - \epsilon)$$

Inserting $\epsilon \beta(E - \epsilon) = S(E) - S(E - \epsilon)$ yields the recursion $^3$$^4$

$$\alpha(E - \epsilon) = \alpha(E) + [\beta(E - \epsilon) - \beta(E)]E$$

where $\alpha(E_{\text{max}}) = 0$ is a convenient choice of the integration constant.

### 3.3 Recursive weight factor estimates

For spin systems with first-order phase transitions the finite size scaling (FSS) behavior is relatively well-known. Provided the steps between system sizes are not too large, it is then possible to get working estimates of the MUCA weights by means of FSS extrapolation from the already simulated smaller systems $^6$. Another method which works well for these systems is patching of overlapping, constraint $^9$ MC simulations. While these approaches seem to
work well for static slowing down, they fail for the dynamic slowing down of spin glass simulations. Then it is recommended to employ a more sophisticated recursion\textsuperscript{10}, as outlined now.

It is advisable to start a recursion for MUCA weights in the disordered region (for which reliable canonical calculations can be performed). For instance,

$$\beta^0(E) \equiv \beta^0(E_{\text{max}}) \text{ e.g. } \beta^0(E_{\text{max}}) = 0$$

Then

$$\beta^{n+1}(E) = \epsilon^{-1} \ln[\hat{H}_0^n(E + \epsilon) / \hat{H}_\beta^n(E)]$$

(1)

where $\hat{H}_x^n(E)$, ($x = 0, \beta$) contains combined information from the runs with $\beta^0(E), ..., \beta^n(E)$:

$$\hat{H}_x^n(E) = \sum_{k=0}^n g^k(E) H^k_x(E)$$

Here $H^k_0(E)$ is the unnormalized histogram obtained from the (short) simulation with $\beta^k(E)$. Further,

$$H^k_\beta(E) = H^k_0(E) e^{-\beta^k(E)}$$

and the factors $g^k(E)$ weight the runs suitably. For instance,

$$g^k(E) = \text{const.} \min[H^k(E + \epsilon), H^k(E)]$$

where the constant follows from the normalization $\sum_k g^k = 1$. For energy regions in which the statistics is (still) insufficient, equation (1) may be supplemented by

$$\beta^{n+1}(E) = \beta^{n+1}(E + \epsilon).$$

An interesting recent idea\textsuperscript{11} is to utilize transition frequencies instead of simple histograms. Finally, connections with adaption and linear response theory have been explored\textsuperscript{12}.

### 3.4 Slowing down

Our typical situation is

$$E_{\text{max}} - E_{\text{min}} \sim V$$

The MUCA optimum for a flat energy distribution is given by a random walk in the energy. This implies a CPU time increase

$$\sim V^2$$
to keep the number of $E_{\text{max}} \rightarrow E_{\text{min}} \rightarrow E_{\text{max}}$ transitions constant. The recursion (1) needs an additional $\sim V^{0.5}$ (optimum) attempts to cover the entire range. It follows:

slowing down $\sim V^{2.5}$ or worse.

Recursion alternative (patching of overlapping constraint\textsuperscript{9} MC simulations):

number of (fixed size) patches $\sim V$.

When results can be obtained by keeping the number of updates per spin (sweeps) in each patch constant, another CPU factor $\sim V$ follows. In this case we can get:

optimal performance $\sim V^2$.

This is still the optimal slowing down when the MUCA parameters can be obtained via FSS extrapolations.

3.5 Related methods

Combining MUCA with multigrid methods has been explored in Ref.\textsuperscript{13} and the cluster version\textsuperscript{7} has already been mentioned. For molecular dynamics, Langevin and hybrid MC variants see Ref\textsuperscript{14}.

The method of expanded ensembles\textsuperscript{15} proposes to enlarge the configuration space by introducing new dynamical variables. In simulated tempering\textsuperscript{16} it is the temperature. A discrete set of weight factors is introduced

$$w_k = e^{-\beta_k E + \alpha_k}, \ k = 1, ..., n, \ \beta_1 < \beta_2 < ... < \beta_{n-1} < \beta_n$$

The transitions

$$(\beta_k, \alpha_k) \rightarrow (\beta_{k-1}, \alpha_{k-1}), (\beta_{k+1}, \alpha_{k+1})$$

are now added to the usual $E \rightarrow E'$ transitions.

Remarks:

- The method works for dynamic but not for static supercritical slowing down, because each member of the discrete set of weight factors samples still a Boltzmann distribution (e.g. it is not suitable for calculating interfacial tensions).

- In the context of massively parallel computer architectures (and beyond) the variant of parallel tempering is particularly promising\textsuperscript{17}. For additional information see the article by Marinari in these proceedings.
Random Cost\textsuperscript{18} sacrifices the exact relationship with the canonical ensemble in favor of having a-priori defined transition probabilities. Assume, we can choose from a discrete set of updates, such that an update implies one of the following energy changes:

\[ \Delta E_i^+, (i = 1, ..., n^+), \Delta E_j^0, (j = 1, ..., n^0) \text{ or } \Delta E_k^-, (k = 1, ..., n^-) \]

where \( \Delta E_i^+ > 0, \Delta E_j^0 = 0 \) and \( \Delta E_k^- < 0 \). It is then easy to define update probabilities \( p_i^+, p_j^0 \text{ and } p_k^- \), \( \sum_i p_i^+ + \sum_j p_j^0 + \sum_k p_k^- = 1 \), such that

\[ \sum_i p_i^+ \Delta E_i^+ = -\sum_k p_k^- \Delta E_k^- \quad (2) \]

holds (but at the extrema). The algorithm performs a random walk in the energy and, hence, samples a broad energy distribution. It is conjectured to be of advantage in optimization problems, where one is mainly interested in minima and less in the canonical ensemble.

4 First-Order Phase Transitions

MUCA simulations are best established for investigations of first-order phase transitions. The range of applications goes from MUCA studies of mathematically ambitious topics to chemistry oriented ones. A MUCA investigation\textsuperscript{19} of the Borgs-Kotecký\textsuperscript{20} FSS theory shows that very strong phase transitions or very large lattices are needed to observe the asymptotic behavior. To give two examples from the chemistry side, an investigation of the coexistence curve of the Lennard-Jones fluid was performed in Ref.\textsuperscript{21} and the liquid-vapor asymmetry in pure fluids was studied in Ref.\textsuperscript{22}.

Most work has focused on calculations of interfacial tensions and an overview is given in the forthcoming.

4.1 2d Potts Models

A pioneering MUCA study was performed for the 2d ten-state Potts model\textsuperscript{4}. Using the histogram method\textsuperscript{23}, the value \( 2f^* = 0.0978(8) \) was found through FSS study of the equation

\[ 2f_L^* = -\frac{1}{L} \ln P_L^\text{min} \quad \text{where} \quad P_L^\text{min} = \min\{P_L(E) | E_L^{\text{max},1} < E < E_L^{\text{max},2}\}. \quad (3) \]

Here \( P_L(E) \) is the normalized energy density at the temperature defined by \( P_L^{\text{max},1} = P_L^{\text{max},2} \). When the first MUCA estimate was published, numerical
estimates of Potts model interfacial tensions disagreed up to one order of magnitude. But, shortly after the exact value was found to be $2f^* = 0.094701...$, see $^{24,25}$ and references therein. Certainly, this helped towards the breakthrough of MUCA methods. Once, the exact result was known, the remaining, small discrepancy could be eliminated by improving the finite volume estimators $^{26}$.

For these simulations the MUCA slowing down is around $\sim V^{2.3}$, i.e. reasonably close to the optimal performance. For related investigations of the seven-state 2d Potts model, see Ref.$^{27,28}$. On the technical side, arguments in favor of using equal weights (instead of equal heights), when applying equation (3) to asymmetric first-order transitions, have been raised $^{29}$.

4.2 2d and 3d Ising Model

Many real physical systems fall into the universality class of the 3d Ising model. Despite its simplicity, it is therefore a very rewarding object to study. Although many of its universal parameters have already been determined with high precision, accurate results for some are still in the making. In particular, there has been recent interest in the universal surface tension and the critical-isotherm amplitude ratios $^{30}$. To obtain them, one needs accurate interfacial tension results below the Curie temperature. Here multimagnetical (MUMA) simulations $^{6}$ have become the enabling technique for Binder’s $^{23}$ histogram method, which was originally proposed in this context.

For the 2d Ising model Onsager’s exact result could be reproduced with good accuracy. However, for the 3d model the temperature dependence of MUMA interfacial tensions has come out fairly erratic. Therefore, the results of Ref.$^{31}$ should be regarded as the up-to-date best estimates. Meanwhile, considerable technical improvements of MUMA calculations are feasible (see also the next subsection) and it seems worthwhile to start off a new, large scale, MUMA 3d Ising model simulation.

4.3 SU(3) Gauge Theory

One is interested in the interfacial tension for the confinement/deconfinement phase transition. The use of MUCA techniques has been explored by Grossmann, Laursen et al. $^{32,33}$. In particular, they noticed that it is suitable to use an asymmetric lattice, $V = L_z L^2 L_t$ with $L_z \geq 3L$. This forces the interfaces into the $L^2$ plane and ensures a flat region for the minimum of equation (3), thus greatly facilitating the extraction of finite-lattice values for the interfacial tension and, consequently, the FSS analysis.
For $SU(3)$ gauge theory the interfacial tension is usually denoted by the symbol $\sigma$ and estimates are conveniently given as multiples of $T_c^3$, where $T_c$ is the deconfinement temperature. Using the conventions of $^{34}$, the estimates of $^{33}$ seem to be

$$\sigma = 0.052(4) T_c^3, \ (L_t = 2) \quad \text{and} \quad \sigma = 0.020(2) T_c^3, \ (L_t = 4)$$

This may be compared with the later estimate by Iwasaki et al. $^{34}$

$$\sigma = 0.02925(22) T_c^3, \ (L_t = 4) \quad \text{and} \quad \sigma = 0.0218(33) T_c^3, \ (L_t = 6)$$

The discrepancy (only $L_t = 4$ can be compared) is presumably due to too small lattice sizes in the MUCA study. Physically, one is interested in the $L_t \to \infty$ limit. Recently, it has been suggested that the the strong $L_t$ dependence can be eliminated by using tadpole improved actions. Beinlich et al. $^{35}$ report

$$\sigma = 0.0155(16) T_c^3, \ (L_t = 2 \ \text{and} \ L_t = 3).$$

### 4.4 Electroweak Phase Transition

Baryon violating processes are unsuppressed for $T > T_c$, where $T_c$ is the electroweak critical temperature. It has been conjectured, that this may allow to explain the baryon asymmetry in nature. Models tie the nucleation rate to the interface tension of the transition. Using an effective scalar field theory $^{37}$ or the full theory $^{38}$, MUCA and related techniques turn out to be useful for simulations at a Higgs mass

$$m_H \approx (35 - 37) \text{GeV},$$

where one deals with a relatively strong first-order transitions, as needed to explain the baryon asymmetry. Unfortunately, it turn out that the transition weakens for higher Higgs masses, see Ref.$^{39}$ for a concise review.

### 5 Systems with Conflicting Constraints

In these systems one encounters large free energy barriers due to disorder and frustrations. MUCA simulations try to overcome the barriers through excursions into the disordered phase. Examples are spin glasses, proteins (see Hansmann in these proceedings), hard optimization problems and others.
5.1 Spin glasses

MUCA studies have so far focused on the simplest, not-trivial prototypes, the $2d$ and $3d$ Edwards-Anderson Ising (EAI) spin glass. Significant progress is achieved with respect to groundstate energy and entropy calculations. However, the slowing down with volumes size is very bad, around $V^4$ or, possibly, exponential. Certain advantages of simulated tempering are claimed in Ref. An uncontroversial one is that the latter approach can easily be vectorized, whereas other issues have straightforward (but yet untested) translations into the MUCA approach. In any case, presently we have no indication that simulated tempering yields a significantly improved slowing down.

5.2 Optimization problems

They occur in engineering, network and chip design, traffic control, and many other situations. General purpose algorithms for their solution are Simulated Annealing and Genetic Algorithms. To those, we may now like to add Multicanonical Annealing and Random Cost. Multicanonical Annealing is a combination of MUCA sampling with variable upper bounds and frequent adaption of parameters. A promising study has been performed for the traveling salesman problem. Up to $N = 10,000$ cities, randomly distributed in the unit square, were considered and scaling of the path length as function of $N$ was investigated. The reported algorithmic performance is so good, that an independent confirmation would be highly desirable.

Two non-trivial applications of the random cost algorithm emerged recently: (i) It was used for training a feed-forward multilayer perceptron, relevant for analyzing high energy physics experimental data. (ii) Topology optimization as needed for the engineering of trusses was studied.

6 Conclusions

Sampling of broad energy distributions allows to overcome supercritical slowing down. This is well established for first-order phase transitions. Systems with conflicting constraints remain, despite some progress, notoriously difficult and for them most hope lies on achieving further algorithmic improvements. Finally, MUCA methods may also be of interest when dealing with second order phase transitions, but so far little experience exists in this direction.
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References

1. G.M. Torrie and J.P. Valleau, *J. Comp. Phys.* **23**, 187 (1977).
2. B. Baumann, *Nucl. Phys.* B **285**, 391 (1987).
3. B. Berg and T. Neuhaus, *Phys. Lett.* B **267**, 249 (1991).
4. B. Berg and T. Neuhaus, *Phys. Rev. Lett.* **69**, 9 (1992).
5. W. Kerler, C. Rebbi and A. Weber, *Nucl. Phys.* B **450**, 452 (1995).
6. B. Berg, et al., *Phys. Rev.* B **47**, 497 (1993); *Z. Phys.* B **90**, 229 (1993).
7. W. Janke and S. Kappler, *Phys. Rev. Lett.* **74**, 212 (1995).
8. B. Hesselbo and R. Stinchcombe, *Phys. Rev. Lett.* **74**, 2151 (1995).
9. G. Bhanot, et al., *Phys. Lett.* B **183**, 331 (1986).
10. B. Berg, *J. Stat. Phys.* **82**, 343 (1996).
11. G.R. Smith and A.D. Bruce, *Phys. Rev.* E **53**, 6530 (1996).
12. T. Munakata and S. Oyama, *Phys. Rev.* E **54**, 4394 (1996).
13. W. Janke and T. Sauer, *Phys. Rev.* E **49**, 3475 (1994).
14. U. Hausmann, et al., *Chem. Phys. Lett.* **259**, 321 (1996).
15. A.P. Lyubartsev, et al., *J. Chem. Phys.* **96**, 1776 (1992).
16. E. Marinari and G. Parisi, *Europhys. Lett.* **19**, 451 (1992).
17. K. Hukushima and K. Nemoto, *J. Phys. Soc. Japan* **65**, 1604 (1996).
18. B. Berg, *Nature* **361**, 708 (1993).
19. A.Billoire, T. Neuhaus and B. Berg, *Nucl. Phys.* B **396**, 779 (1993).
20. C. Borgs, R. Kotecký and S. Miracle-Sole, *J. Stat. Phys.* **62**, 529 (1991).
21. N.B. Wilding, *Phys. Rev.* E **52**, 602 (1995).
22. N.B. Wilding and M. Müller, *J. Chem. Phys.* **102**, 2562 (1995).
23. K. Binder, *Phys. Rev.* A **25**, 1699 (1982).
24. E. Buffenoir and S. Wallon, *J. Phys.* A **26**, 3045 (1993).
25. C. Borgs and W. Janke, *J. de Physique I (Paris)* **2**, 2011 (1992).
26. A. Billoire, T. Neuhaus and B. Berg, *Nucl. Phys.* B **413**, 795 (1994).
27. W. Janke, B. Berg and M. Katoot, *Nucl. Phys.* B **382**, 649 (1992).
28. K. Rummukainen, *Nucl. Phys.* B **390**, 621 (1993).
29. C. Borgs and S. Kappler, *Phys. Lett.* A **171**, 37 (1992).
30. S.-Y. Zinn and M.E. Fisher, *Physica* A **226**, 168 (1996).
31. M. Hasenbusch and K. Pinn, *Physica* A **203**, 189 (1994).
32. B. Grossmann, et al., *Phys. Lett.* B **293**, 175 (1992).
33. B. Grossmann and M.L. Laursen, *Nucl. Phys.* B **408**, 637 (1993).
34. Y. Iwasaki et al., *Phys. Rev.* D **49**, 3540 (1994).
35. B. Beinlich, F. Karsch, and A. Peikert, hep-lat/9608141.
36. H. Meyer-Ortmanns, hep-lat/9608098.
37. F. Karsch, T. Neuhaus, and A. Patkós, *Nucl. Phys.* B **441**, 629 (1995).
38. F. Csikor, et al., *Phys. Lett.* B **357**, 156 (1995).
39. I. Montway, hep-lat/9507024.
40. B. Berg and T. Celik, *Phys. Rev. Lett.* **69**, 2292 (1992).
41. B. Berg, U. Hansmann and T. Celik, PRB **50**, 1644 (1994).
42. W. Kerler and P. Rehberg, *Phys. Rev.* E **50**, 4420 (1994).
43. Y. Lee and M.Y. Choi, *Phys. Rev.* E **50**, R651 (1994).
44. B. Berg, *Comp. Phys. Commun.* **98**, 35 (1996).
45. B. Baumann, preprint, baumann@rzbt.fh-hamburg.de.