High Precision Simulation Techniques
for Lattice Field Theory †

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Abstract

An overview is given over the recently developed and now widely used Monte Carlo algorithms with reduced or eliminated critical slowing down. The basic techniques are overrelaxation, cluster algorithms and multigrid methods. With these tools one is able to probe much closer than before the universal continuum behavior of field theories on the lattice.

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1 Introduction

The interest in statistical systems close to criticality is shared by a large community including condensed matter physicists and particle theorists. An important tool in the study of such systems are numerical experiments in the form of Monte Carlo simulations which complement analytical results that are available for special systems and limiting cases. One of the central problems in such simulations is the degradation of most known simulation algorithms as criticality — the cutoff or continuum limit in quantum field theories describing particles — is approached. The interdisciplinary search of improved techniques is an on-going effort, but it already has yielded some very positive results in recent years some of which we want to briefly review here. Our focus will be on spin systems with variables belonging to continuous manifolds ($\sigma$-models) and on pure lattice gauge theory. This selection thus leaves out the vast field of discrete Ising-like systems\(^1\) as well as the enormous problems (and potential gains from algorithmic improvement) faced in QCD simulations with fermions.\(^2\)

The problem of critical slowing down (CSD) near criticality is schematically described by the dynamical scaling law

$$\tau = c \xi^z. \tag{1}$$

Here $\xi$ is some physical scale or correlation length in lattice units and $\tau$ is a time scale in number of iterations. A $\tau$ and corresponding $z$ can characterize the time scale for equilibration or the rate at which statistically independent estimates for observables of interest are produced. Then for the expectation value of $A$,

$$\langle A[s]\rangle = \frac{1}{Z} \int Ds \; e^{-\beta H[s(x)]} \; A[s], \tag{2}$$

the accuracy in estimating $A$ improves as

$$\delta_A = \sqrt{\text{variance}_A \times 2\tau/# \text{ of iterations}}. \tag{3}$$

In (4) $D s = \prod_x d\mu(s(x))$ means integration over all fields or spins $s(x)$ at lattice sites $x$ with some measure, $Z$ is the partition function and $\beta H[s]$ is the inverse bare coupling or temperature times some action or Hamiltonian.

The algorithms to be described here have been designed to lower $z$ from its “traditional” value of about two for standard local Metropolis methods.
to $z \simeq 1$ or even $z \simeq 0$ in some cases. They thus improve the efficiency of simulations by *one to two powers* of $\xi$.

Beyond the introduction this article will continue with a section on the technique of embedded variables (common to many algorithms), and short descriptions of cluster algorithms, multigrid methods and overrelaxation followed by some conclusions.

2 Updating Embedded Variables

Let us imagine some group of transformations $T \in G$ that act on the configurations $s \doteq \{ s(x) \}$,

$$s \rightarrow Ts,$$

such that the measure is left invariant, $D_s = DTs$. Such transformations can be local, $Ts = \{ t(x)s(x) \}$, and then $t(x)$ is a field similar to $s$ itself with values in local group factors that make up $G$. One may however also consider more global changes of $s$, where $T$ acts for instance on some cluster of spins from $s$ with one and the same rotation. For a given configuration $s$ we can now think of a statistical system with configurations $T \in G$ and an effective or induced Boltzmann factor $\exp(-\beta H[Ts])$ whose simulation can also be considered. Assume now that we have a Monte Carlo algorithm for this system which is characterized by transition probabilities $w(s; T_1 \rightarrow T_2)$ that preserve $\exp(-\beta H[Ts])$ and depend on $s$ only through the effective Boltzmann factor such that $w(Ts; T_1 \rightarrow T_2) = w(s; T_1 T \rightarrow T_2 T)$ holds. Then, if ervalid algorithm for the original field $s(x)$:

- for momentarily fixed $s = s_1$ put $T_1 = Id$ as initial configuration,
- update $T_1 \rightarrow T_2$ with the $w$–algorithm,
- take $s_2 = T_2s_1$ as a new $s$.

To prove this assertion we first note that the overall transition probability is given by

$$W(s_1 \rightarrow s_2) = \sum_T w(s; Id \rightarrow T) \delta(s_2 - Ts_1).$$

\[\text{For simplicity we take a discrete group } G \text{ here; in the continuous case the sum over all elements has to be replaced by an invariant group integration.}\]
We have to show that $W$ preserves the Boltzmann weight $\exp(-\beta H[s])$. To this end we transform

$$\int Ds_1 \ e^{-\beta H[s_1]} \ W(s_1 \to s_2) =$$

$$\int Ds_1 \sum_{T'} e^{-\beta H[Ts_1]} \ w(s_1; \ Id \to T') \ \delta(s_2 - T's_1) =$$

$$\frac{1}{|G|} \int Ds_1 \sum_{T,T'} e^{-\beta H[T's_1]} \ w(s_1; T \to T') \ \delta(s_2 - T's_1) =$$

$$\frac{1}{|G|} \int Ds_1 \sum_{T'} e^{-\beta H[T's_1]} \ \delta(s_2 - T's_1) = e^{-\beta H[s_2]}.$$ (6)

To arrive at the third line changes of variables $s_1 \to Ts_1$ and $T' \to T'T^{-1}$ are carried out and $T$ is averaged over. In the last line we absorbed $T'$ into $s_1$ and the $\delta$-function is used.

In many cases, in particular if $G$ is a lower dimensional manifold than the original configuration space, the moves described are not ergodic. This can often be improved by using families of different embeddings between which one switches in a random or deterministic order. In cases where this is not sufficient one can always blend in conventional update steps to achieve ergodicity.

### 3 Cluster Algorithms

Cluster algorithms\(^3\) for continuous spins are an example of the successful use of variables. Their drawback has been up to now that the $O(n)$ invariant $n$-vector models are the only continuous variable $\sigma$-models where they are powerful.\(^5\) Here however, according to accumulated numerical evidence\(^5\), they really achieve $z \simeq 0$ with even a very small coefficient $c$ in (1). With the additional advantage of variance reduced estimators for Green functions, these models have become an ideal testing ground for nonperturbative physics\(^6\), in particular in two dimensions, where they are asymptotically free for $n \geq 3$. Also the xy-model ($n = 2$) is of great interest\(^7\) as it allows for checks of the Kosterlitz Thouless scenario. We therefore now specialize our general setup, \(^\dagger\)

\(^\dagger\)There are principal reasons for this limitation which come close to a no-go theorem.\(^4\)
Eq. (2), to the $O(n)$ models, where

$$s(x) \in \mathbb{R}^n, \quad D_s = \prod_x d^n s(x) \delta(s(x)^2 - 1), \quad -H[s] = \sum_{<xy>} s(x) \cdot s(y). \quad (7)$$

The key to efficient cluster algorithms is the embedding of Ising spins and the use of global update techniques for them. A family of embeddings is labelled by an $n$-component unit vector $r$ of the same type as the local spins. The group involved is $G_r \simeq \mathbb{Z}_2^\#\text{sites}$ corresponding to one Ising spin $\sigma(x) = \pm 1$ on each site, $T \leftrightarrow \{\sigma(x)\}$. They act as reflections,

$$s' = Ts, \quad s'(x) = s_{\perp}(x) + \sigma(x)s_{\parallel}(x), \quad (8)$$

where $\perp$ and $\parallel$ refer to the $r$-direction. The induced Hamiltonian

$$-H[Ts] = \sum_{<xy>} r \cdot s(x) r \cdot s(y) \sigma(x)\sigma(y) + \text{terms independent of } \sigma \quad (9)$$

is recognized to describe a ferromagnetic Ising model with random bond strengths $J_{<xy>} = r \cdot s(x) r \cdot s(y)$. When they are multiplied along closed loops the result is always positive or zero due to their factorized form, which shows the absence of frustration. We also note that there is no magnetic field coupling to $\sigma$. This can be regarded as being due to the reflections in (8) being part of the $O(n)$ global symmetry which leads to a global $\mathbb{Z}_2$ invariance for $\sigma$. For these embedded random systems the Swendsen-Wang algorithm\textsuperscript{8} or its single cluster variant\textsuperscript{3} work very well, actually better than in the standard Ising model where some remaining CSD is still detectable.

The algorithm just described is ergodic if $r$ is chosen at random such that all directions can appear. In practical realizations it is usually convenient to always take $r = (1, 0, \ldots, 0)$. Then the embedding requires fewer operations, and ergodicity is restored by globally $O(n)$-transforming the whole configuration with a random rotation or reflection after a certain number of updates.

4 Multigrid Techniques

Multigrid Monte Carlo (MGMC) techniques have been proposed\textsuperscript{9} to eliminate CSD by allowing for efficient moves of a critical system on all scales.
They work well on nearly gaussian systems as they do in the related problem of linear difference equations where the method has made its first appearance. Here we will not review the truly recursive MGMC approach but a simpler unigrid variant that was proposed recently. It has become the optimal method for $\sigma$-models other than the $O(n)$ family.

We now present the method for the $O(3)$-model. The actual updates are performed here (and in realizations for other $\sigma$-models) on embedded $U(1)$ spins of the xy-model type. To an $O(3)$ generator corresponding to some rotation, as for example

$$i\lambda = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

we couple local angles $\alpha(x)$ by

$$T_s = \{e^{-i\alpha(x)}s(x)\}.$$

This induces a Hamiltonian for $\alpha(x)$,

$$-H[T s] = \sum_{<xy>} \text{Re} \left( J_{<xy>} e^{i(\alpha(x) - \alpha(y))} \right) + \text{terms independent of } \alpha$$

with complex bond strengths

$$J_{<xy>} = (s^1(x) + is^2(x))(s^1(y) - is^2(y)) = J^*_{<yx>}$$

where $s^a, a = 1, 2, 3$, denotes the components of $s$. The random bonds generated for the embedded xy-model are again ferromagnetic due to their factorized form. As for $U(1)$ gauge fields their orientation has to be properly taken into account, of course.

We now need an algorithm for $\alpha(x)$. For the version of MGMC of Ref. 12 elementary moves are performed on $B \times B \times \ldots \times B$ subblocks of the lattice. For such blocks one has a priory fixed profiles of kernels $K(x)$ that vanish outside the block and are smooth. Possible choices in arbitrary dimensions are pyramids or the lowest mode sine waves with the block as a cavity. The kernels appear in the nonlocal Metropolis proposals

$$\{\alpha(x)\} \rightarrow \{\alpha(x) + \Psi K(x)\}.$$
These are accepted or rejected in the usual way, and $\Psi$ is drawn from a symmetric distribution with a width adjusted for reasonable acceptance. For a lattice of length $L$, which should be a power of two, one has to hierarchically cover the lattice with blocks of sizes $B = L/2, L/4, \ldots, 1$ with the last choice producing just local updates. It has turned out to be important that either the superimposed block lattice or equivalently the field configuration is randomly translated between updates, such that the block boundaries are not at fixed positions. Furthermore the generator $\lambda$ is randomized to achieve ergodicity.

For $O(n)$ models this MGMC algorithm is presumably inferior to cluster methods, although detailed comparisons would be somewhat hardware dependent. The importance of the technique derives however from the fact, that it can also be used for $CP^n$-models and for $SU(n)$ valued spins. The main change is that appropriate generators (from $U(n)$ and $SU(n)$ respectively) have to be substituted for $\lambda$. The resulting embedded $U(1)$ system now can have frustration depending on the configuration of the “background” spins $s$. Practical tests for the $SU(3) \times SU(3)$ chiral model and for the $CP^3$ system have shown that these frustrations do not seriously slow down the evolution.\textsuperscript{13} In all three cases $z = 0.2(1)$ has been found.

5 Overrelaxation

In contrast to the two previous algorithms overrelaxation (OR) achieves an improvement (down to $z \approx 1$) with still local updates only, and hence it is as fast or even somewhat faster per sweep than standard algorithms. It also immediately carries over to gauge fields. We now present OR in its “hybrid” form that found many applications recently rather than the original “tunable” version\textsuperscript{14}. We consider the local update problem at site $x$ with local Boltzmann weight

$$e^{\beta s(x) \cdot M(x)}$$

where

$$M(x) = \sum_{y=\text{n.n. of } x} s(y),$$

again for an $O(n)$ model spin for illustration. A local heatbath procedure amounts to choosing a new $s(x)$ independently of the old one with the weight \textsuperscript{(15)}. For OR we need additional microcanonical steps producing transitions $s_1(x) \rightarrow s_2(x)$ such that
• \( s_1(x), s_2(x) \) have the same local weight \((15)\) and thus the energy is unchanged,

• \( s_1(x), s_2(x) \) are as far from each other as possible.

For our example this principle leads to the change

\[
s_2(x) = -s_1(x) + 2 \frac{M \cdot s_1(x)}{M^2}.
\]

(16)

Experience has shown that both for vectorization and for the nonuniversal it is best to group the local updates such as to do a maximum number of independent ones in parallel, which usually amounts to checkerboard ordering. Now an OR iteration consists of \( N \) microcanonical sweeps followed by one heatbath or other standard ergodic step. From exact gaussian analysis\(^{15}\) and from numerical experiments\(^{16}\) it is known that to achieve \( z \approx 1 \) it is necessary do let \( N \) grow proportional to \( \xi \) as criticality is approached. Often \( N = \xi \) is a reasonably good trial value. The goal is to achieve a roughly constant autocorrelation time when measured in iterations which implies \( z \approx 1 \) when referring to sweeps.

In particular, this kind of OR is the present method of choice for SU(2) lattice gauge fields (either fundamental or embedded to move SU(3) fields). The local problem for a link variable \( U_\mu(x) \in SU(2) \) coincides with the \( O(4) \) case when \( SU(2) \) matrices are expanded in terms of the unit- and the Pauli-matrices.

We close with the example of a recent simulation of the \( SU(2) \) gauge theory\(^{17}\) where it was possible to determine the relation between \( \tau \) and a scale in lattice units for a whole range of scales as shown in Fig. 1. In this study a renormalized coupling constant was held fixed which is equivalent to a finite size scaling limit at fixed \( L \sqrt{K} \) with the string tension \( K \) assuming the rôle of a correlation length. The time \( \tau \) refers to independently estimating the renormalized coupling. The line in the plot represents a fit with the form \((1)\) giving \( z = 1.0(1) \) and \( c = 0.5(1) \). For further details on algorithmic and physical aspects of this work we have to refer to Ref. 17.

### 6 Conclusions

We have presented some of the accelerated algorithms for the Monte Carlo simulation of spin and gauge theories that have been discovered and tested
in recent years. As a result, critical continuum behavior can be studied now much more accurately, especially in two and three dimensions. In four dimensions, which is the most interesting case for particle physics, the situation will become similar as larger systems will be studied on future computers. In the presence of Goldstones modes, the new techniques are crucial already now.

When algorithms of the multigrid type with \( z < 1 \) will be found for gauge theories, it will strongly depend on the overhead inflicted, at which system size they really become profitable. In simulations of the \( CP^3 \) model, for instance, it has been found that on vector machines the crossover between OR and MGMC occurs only for correlation lengths \( \xi = 20 \ldots 30,^{13,18} \)

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