Theoretical Analysis of Acceptance Rates in Multigrid Monte Carlo

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Abstract

We analyze the kinematics of multigrid Monte Carlo algorithms by investigating acceptance rates for nonlocal Metropolis updates. With the help of a simple criterion we can decide whether or not a multigrid algorithm will have a chance to overcome critical slowing down for a given model. Our method is introduced in the context of spin models. A multigrid Monte Carlo procedure for nonabelian lattice gauge theory is described, and its kinematics is analyzed in detail.

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1 Introduction

Multigrid Monte Carlo algorithms were introduced to overcome critical slowing down (CSD) \[1\]. For some interacting models, numerical experiments showed that the dynamical critical exponent $z$ was indeed substantially reduced \[2\]. For other models, still $z \approx 2$ was found \[3\].

Therefore, an improved theoretical understanding of these algorithms is desirable. We study the kinematics of multigrid Monte Carlo by investigating the scale dependence of acceptance rates for nonlocal Metropolis updates. A simple criterion for the possible success of a multigrid algorithm is given. Our analysis is also useful for the design of new multigrid algorithms for nonabelian gauge fields.

2 Multigrid Monte Carlo

First we consider models with partition functions

$$Z = \int \prod_{x \in \Lambda_0} d\phi_x \exp(-\mathcal{H}(\phi))$$

(1)

on cubic $d$-dimensional lattices $\Lambda_0$. We shall use dimensionless spin variables. Nonlocal Monte Carlo updates are defined as follows: Divide the fundamental lattice $\Lambda_0$ in cubic blocks of size $l^d$ (e.g. $l = 2$). This defines a block lattice $\Lambda_1$. By iterating this procedure one gets a hierarchy of block lattices $\Lambda_0, \Lambda_1, \ldots, \Lambda_K$. We denote block lattice points in $\Lambda_k$ by $x'$. Block spins $\Phi_{x'}$ are defined on block lattices $\Lambda_k$. They are averages of the fundamental field $\phi$ over blocks of side length $L_B = l^k$:

$$\Phi_{x'} = L_B^{(d-2)/2} L_B^{-d} \sum_{x \in x'} \phi_x.$$

(2)

A nonlocal change of the configuration $\phi$ consists of a shift

$$\phi_x \rightarrow \phi_x + s \psi_x,$$

(3)

where $s$ is a real parameter. The shape of the nonlocal change is determined by the “coarse-to-fine interpolation kernel” $\psi$ that obeys the constraint

$$L_B^{-d} \sum_{x \in x'} \psi_x = L_B^{(2-d)/2} \delta_{x', x_0}.$$

(4)

Note that the effect of (3) on $\Lambda_k$ is $\Phi_{x'} \rightarrow \Phi_{x'} + s$ for $x' = x'_0$, whereas $\Phi_{x'}$ remains unchanged on the other blocks. The simplest $\psi$ is a piecewise constant kernel: $\psi_x = L_B^{(2-d)/2}$ if $x \in x'_0$, and 0 else. One can also use smooth kernels that avoid large energy costs from the block boundaries.

The $s$-dependent Metropolis acceptance rate for such proposals is given by

$$\Omega(s) = \langle \min[1, \exp(-\Delta \mathcal{H})] \rangle,$$

(5)
where $\Delta \mathcal{H} = \mathcal{H}(\phi + s\psi) - \mathcal{H}(\phi)$. The starting point of our acceptance analysis is
the approximation formula \[4, 5, 6\]

$$\Omega(s) \approx \text{erfc} \left( \frac{1}{2} \sqrt{h_1} \right). \quad (6)$$

Here, $h_1 = \langle \Delta \mathcal{H} \rangle$ denotes the average change in the fundamental Hamiltonian.
Generally, the formula yields precise estimates that are confirmed by the acceptance rates directly measured in Monte Carlo simulations \[5, 6\]. We will use (6) to predict the acceptance rate $\Omega(s)$ for interacting models. Let us first discuss free massless field theory with action $\mathcal{H}(\phi) = \frac{1}{2} \langle (\phi, -\Delta \phi) \rangle$. Here, we obtain the exact result

$$\Omega(s) = \text{erfc} \left( \sqrt{\frac{\alpha}{8}} |s| \right), \quad (7)$$

with $\alpha = (\psi, -\Delta \psi)$. In $d$ dimensions one finds $\alpha = 2dL_B$ for piecewise constant kernels, and, for smooth kernels, $\alpha \to \text{const if } L_B \gg 1$. (For a systematic study of different kernels see ref. \[6\].) As a consequence, in massless free field theory, to maintain a constant acceptance rate (of, say, 50 percent) the amplitudes $s$ have to be scaled down like $L_B^{-1/2}$ for piecewise constant kernels, whereas for smooth kernels the acceptance rates do not depend on the block size. (At least for free field theory, the disadvantage of the piecewise constant kernels can be compensated for by using a W-cycle instead of a V-cycle. Smooth kernels can be used only in V-cycle algorithms.)

### 3 Spin Models

Now we discuss multigrid procedures for spin models. The kinematical analysis is a comparison of the scale dependence of acceptance rates for interacting models with the behavior in free field theory, where CSD is known to be eliminated by a multigrid algorithm.

As an example we consider the 2-dimensional Sine Gordon model defined by the Hamiltonian

$$\mathcal{H}(\phi) = \frac{1}{2\beta} (\phi, -\Delta \phi) - \zeta \sum_x \cos \phi_x. \quad (8)$$

The model undergoes a (Kosterlitz-Thouless) phase transition at $\beta_c$, and $\beta_c \to 8\pi$ for $\zeta \to 0$. In the massless phase ($\beta > \beta_c$), the long wavelength excitations are spin waves. Since multigrid is an efficient method to accelerate spin waves in free massless field theory, one might expect that multigrid should be also the right method to fight CSD in the massless phase of the Sine Gordon model. But this expectation is wrong: For $h_1$ we find the expression

$$h_1 = \frac{\alpha}{2\beta} s^2 + \zeta C \sum_x [1 - \cos(s\psi_x)], \quad (9)$$

with $C = \langle \cos \phi_x \rangle$. Expanding for small $s$, we find that the second term in (9) behaves like $\sim s^2 \sum_x \psi_x^2$, like a “mass” term in the kernel $\psi$. Since $\sum_x \psi_x^2$ is proportional to the block volume $L_B^2$ for piecewise constant and for smooth kernels,
one therefore has to face a dramatic decrease of acceptance when the blocks become large. A constant acceptance rate can only be achieved when the proposed steps $s$ are scaled down like $L_B^{-1}$. It is therefore unlikely that any multigrid algorithm - based on nonlocal updates of the type discussed here - will be successful for this model.

Analyzing multigrid algorithms, we found two classes of models \[5, 6\]. For 2d Sine Gordon and $\phi^4$ theory, $s$ has to be rescaled like $L_B^{-1}$ for piecewise constant and for smooth kernels, whereas for massless free field theory, the 2d XY model, the 2d $O(N)$ nonlinear $\sigma$-model and $U(1)$ lattice gauge theory, one can achieve $L_B$-independent acceptance rates choosing smooth kernels.

For almost all models of the second class, at least a substantial reduction of CSD could be achieved \[4\]. An exception is the 2d XY model in the vortex phase. There $z \approx 1.4$ was found \[7\]. This shows that good acceptance rates alone are not sufficient to overcome CSD.

The results of the analysis are consistent with the following rule: Sufficiently high acceptance rates for a complete elimination of CSD can only be expected if $h_1 = \langle \mathcal{H}(\phi + s\psi) - \mathcal{H}(\phi) \rangle$ contains no algorithmic “mass” term $\sim s^2 \sum_x \psi_x^2$.

## 4 Nonabelian Gauge Fields

We study 4-dimensional $SU(2)$ lattice gauge theory with standard Wilson action

$$\mathcal{H}(U) = \beta \sum_P [1 - \frac{1}{2} \text{Tr} U_P] \quad .$$

The $U_P$ are the usual path ordered products around plaquettes $P$.

### 4.1 Covariant nonlocal update proposal

We want to update only link variables $U_{x,\tau}$ pointing in a selected direction $\tau$. Then only $U_{x,\tau}$ variables in the same 3-dimensional slice $\Lambda^x_\tau = \{x \in \Lambda_0 \mid x_\tau = t\}$ are coupled (when all other link variables $U_{x,\mu}$ with $\mu \neq \tau$ are kept fixed). Regard the $U_{x,\tau}$ variables as spins. We then perform updates for a 3-dimensional spin model in a disordered background field given by the fixed link variables in the directions $\mu \neq \tau$.

Now build 3-dimensional blocks $x'_{o}$ of size $L_B^3$ that are contained in the slice $\Lambda^x_\tau$. Nonlocal update proposals will be global rotations of all link variables $U_{x,\tau}$ attached to sites $x$ inside the block $x'_{o}$ by multiplying them with an $SU(2)$-matrix.

Such global rotations only make sense if we have a certain smoothness of gauge fields inside the slice $\Lambda^x_\tau$. We define a gauge transformation $g$ by the Coulomb gauge condition

$$G_C(U, g) = \sum_{(x,x+\hat{\mu}) \in \Lambda^x_\tau} \text{Tr}(g_x U_{x,\mu} g_{x+\hat{\mu}}^*) \overset{!}{=} \text{max}. \quad (11)$$

If we actually performed this gauge transformation $U_{x,\mu}^g = g_x U_{x,\mu} g^*_{x+\hat{\mu}}$ we would end up with the gauge fields fixed to the Coulomb gauge. However, we will use the
transformation \( g \) only to achieve a smooth rotation of the \( U_{x,\tau} \) variables inside the block. This smooth rotation is defined as follows:

Propose new link variables \( U'_{x,\tau} \) by

\[
U_{x,\tau} \rightarrow U'_{x,\tau} = g_x^* R_x g_x U_{x,\tau},
\]

with

\[
R_x(\vec{n}, s) = \cos(s\psi_x/2) + i \sin(s\psi_x/2) \vec{n} \cdot \vec{\sigma}.
\]

\( s \) is a uniformly distributed random number from the interval \([-\varepsilon, \varepsilon]\), \( \vec{n} \) is a 3-dimensional random unit vector, and \( \vec{\sigma} \) are the Pauli matrices. \( \psi \) again denotes a kernel normalized as in (4). Finally calculate the associated change of the Hamiltonian \( \Delta H \) and accept the proposed link variables with probability \( \min[1, \exp(-\Delta H)] \).

One can show that this is a valid algorithm [6]. For the detailed balance condition it is crucial to ensure that the updates are reversible. We have to get the same \( g \) before and after the move \( U_{x,\tau} \rightarrow U'_{x,\tau} \). This is fulfilled here, since only link variables \( U_{x,\mu} \) with \( \mu \neq \tau \) enter in the Coulomb gauge functional.

Note that we do not have to extremize the gauge functional perfectly. If we always use the same algorithm (e.g. a given number of relaxation sweeps starting from \( g = 1 \)), we will always get the same \( g \) and the nonlocal update is reversible.

| lattice size | \( \beta \) | \( m_D \) | \( \sqrt{\kappa} \) | \( m_{0+} \) | \( m_D/\sqrt{\kappa} \) | \( m_D/m_{0+} \) |
|--------------|--------------|--------------|--------------|-------------|-----------------|-----------------|
| 16^4         | 2.4          | 0.4955(2)    | 0.258(2)     | 0.94(3)     | 1.92            | 0.53            |
| 20^4         | 2.6          | 0.4650(2)    | 0.125(4)     | 0.52(3)     | 3.72            | 0.89            |

Estimates for physical masses are taken from ref. [8].

4.2 Acceptance analysis for \( SU(2) \)

Now we are going to check whether our proposal has a chance to overcome CSD. For the quantity \( h_1 = \langle \Delta H \rangle \) that enters in the approximation formula (6) for the acceptance rates, we get (using piecewise constant \( \psi \))

\[
h_1 = 3A(L_B - 1)L_B^2 \sin^2(sL_B^{-1/2}/2) + 6P L_B^2[1 - \cos(sL_B^{-1/2}/2)],
\]

with

\[
A = -\frac{\beta}{2} \langle \text{Tr}((\vec{n} \cdot \vec{\sigma} U^g_{x,\mu} \vec{n} \cdot \vec{\sigma} - U^g_{x,\mu}) H^g_{x,\mu}) \rangle,
\]

\[
H^g_{x,\mu} = U_{x+\mu,\tau} U^g_{x+\tau,\mu} U_{x,\tau}^*, \text{ and } P = \beta/2 \langle \text{Tr}U^g_\tau \rangle.
\]

If we expand \( h_1 \) for small \( s \), we see that the second term (coming from plaquettes that have one link in common with the block) is linear in \( L_B \), the usual surface energy with piecewise constant kernels.
But the first term (coming from plaquettes that are entirely inside the block) is again a “mass” term: it behaves like $\sim A s^2 L_B^2$.

Let us discuss the origin of this term in more detail: In the weak coupling limit $\beta \to \infty$ we have only pure gauges, i.e. $U_{x,\mu}^g \to 1$ (with the gauge transformation $g$ defined as above). Then the difference of the two terms contributing to $A$ vanishes, and $A \to 0$. In this limit the unwanted mass term vanishes, and the acceptance rates behave just like in massless free field theory.

For finite $\beta$, however, $U_{x,\mu}^g \neq 1$ and therefore $A > 0$ because of the disorder of the gauge fields inside the block. Motivated by this, we identify the square root of $A$ with a “disorder mass” $m_D = \sqrt{A}$. This disorder mass term will dominate the average energy change $h_1$ for large $L_B$

$$h_1 = \langle \Delta H \rangle \underset{L_B \gg 1}{\sim} m_D^2 s^2 L_B^2.$$ (16)

Close to criticality one might hope that $m_D$ scaled with physical masses in the theory, say, the square root of the string tension $\kappa$ or the lowest glue ball mass $m_{0+}$. Then, the fluctuations created by the algorithm would behave similar to the physical fluctuations, and we would expect the algorithm to behave well. But we have to face the fact that $m_D$ will be dominated by the local disorder and decreases much slower than the physical masses in the system. This will be examined now.

### 4.3 Monte Carlo study of $m_D$

We computed $m_D$ for several values of $\beta$. To maximize $G_C$ we used 50 Gauss-Seidel relaxation sweeps. Tests showed that increasing the number of relaxation sweeps beyond 50 hardly lowered $m_D$ any further.

In table 1 we display the ratios of the disorder mass $m_D$ with physical masses. The results show that the disorder mass is nearly independent of $\beta$ in the range studied, whereas the physical masses decrease by roughly a factor of two. In order to keep constant acceptance rate for increasing block size $L_B$, one again has to rescale $s \sim 1/L_B$. Updating on large blocks gets essentially ineffective, and we have to expect CSD for this algorithm.

### 4.4 Implementation and Test

We implemented and tested the algorithm with 3-dimensional blocks using piecewise constant kernels and a W-cycle as described in ref. We did not observe any substantial speed up compared to a local heat bath algorithm (not even a constant factor). This is in agreement with our prediction that updates on larger blocks are not efficient.

### Conclusions

The kinematical mechanism that leads to a failure of multigrid algorithms is well described by our analysis. We hope that a better understanding of this problem can
lead to improved multigrid algorithms that can overcome kinematical obstructions stemming from an algorithmic “mass” term.

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