Monte Carlo Overrelaxation for $SU(N)$ Gauge Theories

Philippe de Forcrand$^{1,2}$ and Oliver Jahn$^{1,3}$

1 Institute for Theoretical Physics, ETH, CH-8093 Zürich, Switzerland
2 CERN, Physics Department, TH Unit, CH-1211 Geneva 23, Switzerland
3 Center for Theoretical Physics, MIT, Cambridge, MA 02139, USA

forcrand@phys.ethz.ch
jahn@mit.edu

Summary. The standard approach to Monte Carlo simulations of $SU(N)$ Yang-Mills theories updates successive $SU(2)$ subgroups of each $SU(N)$ link. We follow up on an old proposal of Creutz, to perform overrelaxation in the full $SU(N)$ group instead, and show that it is more efficient.

The main bottleneck in Monte Carlo simulations of QCD is the inclusion of light dynamical fermions. For this reason, algorithms for the simulation of Yang-Mills theories have received less attention. The usual combination of Cabibbo-Marinari pseudo-heatbath [1] and Brown-Woch microcanonical overrelaxation [2] of $SU(2)$ subgroups is considered satisfactory. However, the large-$N$ limit of QCD presents a different perspective. Fermionic contributions are suppressed as $1/N$, so that studying the large-$N$ limit of Yang-Mills theories is interesting in itself. High precision is necessary to isolate not only the $N \to \infty$ limit, but also the leading $1/N$ correction. Such quantitative studies by several groups are underway [3]. They show that dimensionless combinations of the glueball masses, the deconfinement temperature $T_c$, and the string tension $\sigma$ approach their $N \to \infty$ limit rapidly, with rather small corrections $\sim 1/N^2$, even down to $N = 2$. The prospect of making $O(1/N^2) \sim 10\%$, or even $O(1/N) \sim 30\%$ accurate predictions for real-world QCD is tantalizing. Numerical simulations can guide theory and help determine the $N = \infty$ “master field”.

Already, an old string prediction $T_c/\sqrt{\sigma}(N = \infty) = \sqrt{\frac{1}{\pi(d-2)}}$, first dismissed by the author himself because it disagreed with Monte Carlo data at the time [4], appears to be accurate to within $1\%$ or better. Proposals about the force between charges of $k$ units of $Z_N$ charge, so-called $k$-string tensions, can be confronted with numerical simulations, which may or may not give support to connections between QCD and supersymmetric theories [5]. Efficient algorithms for $SU(N)$ Yang-Mills theories are highly desirable.

Here, we revive an old, abandoned proposal of Creutz [6], to perform overrelaxation in the full $SU(N)$ group, and show its superiority over the traditional $SU(2)$ subgroup approach$^4$.

$^4$ Global updates, of Hybrid Monte Carlo type, are not considered here, because they were shown to be $O(100)$ times less efficient than local ones for $SU(3)$ in [7].
1 State of the Art

We consider the problem of updating a link matrix \( U \in SU(N) \), from an old value \( U_{\text{old}} \) to \( U_{\text{new}} \), according to the probability density

\[
P(U) \propto \exp\left(\beta \frac{1}{N} \text{Re} \text{Tr} X^\dagger U\right).
\]

\( \text{Re} \text{Tr} X^\dagger U \) is the “local action”. The matrix \( X \) represents the sum of the “staples”, the neighboring links which form with \( U \) a closed loop contributing to the action. This is the situation for the Wilson plaquette action, or for improved actions (Symanzik, Iwasaki, ...) containing a sum of loops all in the fundamental representation. Higher representations make the local action non-linear in \( U \). This typically restricts the choice of algorithm to Metropolis, although the approach below can still be used to construct a Metropolis candidate (as e.g. in [8]). Thus, \( X \) is a sum of \( SU(N) \) matrices, i.e. a general \( N \times N \) complex matrix.

Three types of local Monte Carlo algorithms have been proposed:

- **Metropolis**: a random step \( R \) in \( SU(N) \) is proposed, then accepted or rejected. Thus, from \( U_{\text{old}} \), a candidate \( U_{\text{new}} = RU_{\text{old}} \) is constructed. To preserve detailed balance, the Metropolis acceptance probability is

\[
P_{\text{acc}} = \min(1, \exp(\beta \frac{1}{N} \text{Re} \text{Tr} X^\dagger(U_{\text{new}} - U_{\text{old}})))
\]

Acceptance decreases as the stepsize, measured by the deviation of \( R \) from the identity, increases. And an \( N \times N \) matrix multiplication must be performed to construct \( U_{\text{new}} \), which requires \( O(N^3) \) operations. This algorithm is simple but inefficient, because the direction of the stepsize is random. By carefully choosing this direction, a much larger step can be taken as we will see.

- **Heatbath**: a new matrix \( U_{\text{new}} \) is generated directly from the probability density \( P(U) \) Eq.(1). This is a manifest improvement over Metropolis, since \( U_{\text{new}} \) is completely independent of \( U_{\text{old}} \). However, sampling \( P(U) \) requires knowledge of the normalization on the right-hand side of Eq.(1). For \( SU(2) \), the simple algorithm of [9] has been perfected for large \( \beta \) [10]. For \( SU(3) \), a heatbath algorithm also exists [11], although it can hardly be called practical. For \( SU(N), N > 2 \), one performs instead a pseudo-heatbath [1]. Namely, the matrix \( U_{\text{old}} \) is multiplied by an embedded \( SU(2) \) matrix \( R = 1_N - 2 \otimes R_{SU(2)} \), chosen by \( SU(2) \) heatbath from the resulting probability \( \propto \exp(\beta \frac{1}{N} \text{Re} \text{Tr} (X^\dagger U_{\text{old}}) R) \). Note that computation of the 4 relevant matrix elements of \( (X^\dagger U_{\text{old}}) \) requires \( O(N) \) work. To approach a real heatbath and decrease the correlation of \( U_{\text{new}} = U_{\text{old}} R \) with \( U_{\text{old}} \), a sequence of \( SU(2) \) pseudo-heatbaths is usually performed, where the \( SU(2) \) subgroup sweeps the \( \frac{N(N-1)}{2} \) natural choices of off-diagonal elements of \( \hat{U} \). The resulting amount of work is then \( O(N^3) \), which remains constant relative to the computation of \( X \) as \( N \) increases.

- **Overrelaxation**: Adler introduced stochastic overrelaxation for multi-quadratic actions [12]. The idea is to go beyond the minimum of the local action and multiply this step by \( \omega \in [1, 2] \), “reflecting” the link \( U_{\text{old}} \) with respect to the action minimum. This results in faster decorrelation, just like it produces faster convergence in linear systems. In fact, as in the latter, infrared modes are accelerated at the expense of ultraviolet modes, as explained in [13]. The overrelaxation parameter \( \omega \) can be tuned. Its optimal value approaches 2 as the dynamics becomes more critical. In this limit, the UV modes do not evolve and the local action is conserved, making
the algorithm microcanonical. In practice, it is simpler to fix $\omega$ to 2, and alternate overrelaxation with pseudo-heatbath in a tunable proportion (typically 1 HB for 4-10 OR, the latter number increasing with the correlation length). In $SU(2)$, this strategy has been shown to decorrelate large Wilson loops much faster than a heatbath [14], with in addition some slight reduction in the amount of work. It is now the adopted standard. For $SU(N)$, one performs $\omega = 2$ microcanonical overrelaxation steps in most or all $SU(2)$ subgroups, as described in [2].

The $SU(2)$ subgroup overrelaxation of Brown and Woch is simple and elegant. Moreover, it requires minimal changes to an existing pseudo-heatbath program. But it is not the only possibility. Creutz [6] proposed a general overrelaxation in the $SU(N)$ group. And Patel [15] implemented overrelaxation in $SU(3)$, whose efficiency was demonstrated in [7]. Here, we generalize Patel’s method to $SU(N)$.

2 $SU(N)$ Overrelaxation

It may seem surprising at first that working with $SU(N)$ matrices can be as efficient as working on $SU(2)$ subgroups. One must bear in mind that the calculation of the “staple” matrix $X$ requires $O(N^3)$ operations, since it involves multiplying $N \times N$ matrices. The relative cost of updating $U$ will remain bounded as $N$ increases, if it does not exceed $O(N^3)$ operations. An update of lesser complexity will use a negligible fraction of time for large $N$, and can be viewed as a wasteful use of the staple matrix $X$. Therefore, it is a reasonable strategy to spend $O(N^3)$ operations on the link update. A comparison of efficiency should then be performed between (i) an update of all $\frac{N(N^2-1)}{2}$ $SU(2)$ subgroups, one after the other, following Cabibbo-Marinari and Brown-Woch; (ii) a full $SU(N)$ update, described below, involving a polar decomposition of similar $O(N^3)$ complexity. One may still worry that (ii) is unwise because the final acceptance of the proposed $U_{\text{new}}$ will decrease very fast as $N$ increases. Fig. 1 addresses this concern: the acceptance of our $SU(N)$ update
scheme decreases in fact very slowly with \( N \), and remains almost 1 for all practical \( N \) values.

We now explain how to perform \( SU(N) \) overrelaxation, along the lines of [6]. The idea of overrelaxation is to go, in group space, in the direction which minimizes the action, but to go beyond the minimum, to the mirror image of the starting point. If \( \hat{X} \) is the \( SU(N) \) group element which minimizes the action, then the rotation from \( U_{\text{old}} \) to \( \hat{X} \) is \((\hat{X}U_{\text{old}})^{-1}\). Overrelaxation consists of applying this rotation twice:

\[
U_{\text{new}} = (\hat{X}U_{\text{old}})^{-1}U_{\text{old}} = \hat{X}U_{\text{old}}^\dagger \hat{X}
\]

\( U_{\text{new}} \) should then be accepted with the Metropolis probability Eq. (2). The transformation Eq. (3) from \( U_{\text{old}} \) to \( U_{\text{new}} \) is an involution (it is equal to its inverse). From this property, detailed balance follows.

Note that this holds for any choice of \( \hat{X} \) which is independent of \( U_{\text{new/old}} \), resulting always in a valid update algorithm. Its efficiency, however, depends on making a clever choice for \( \hat{X} \). The simplest one is \( \hat{X} = 1 \) \( \forall X \), but the acceptance is small. Better alternatives, which we have tried, build \( \hat{X} \) from the Gram-Schmidt orthogonalization of \( X \), or from its polar decomposition. We have also considered applying Gram-Schmidt or polar decomposition to \( X^\dagger \) or to \( X^\ast \). In all cases, a subtle issue is to make sure that \( U_{\text{new}} \) is indeed special unitary (\( \det U_{\text{new}} = 1 \)), which entails cancelling in \( \hat{X} \) the phase usually present in \( \det X \). The best choice for \( \hat{X} \) balances work, Metropolis acceptance and effective stepsize. Our numerical experiments have led us to the algorithm below, based on the polar decomposition of \( X \), which comes very close to finding the \( SU(N) \) matrix which minimizes the local action. Note that Narayanan and Neuberger [16] have converged independently to almost the same method (they do not take Step 3 below).

### 2.1 Algorithm

1. Perform the Singular Value Decomposition (SVD) of \( X \): \( X = U\Sigma V^\dagger \), where \( U \) and \( V \in U(N) \), and \( \Sigma \) is the diagonal matrix of singular values \( \sigma_i (\sigma_i = \sqrt{\lambda_i}) \), where the \( \lambda_i \)'s are the eigenvalues of the non-negative Hermitian matrix \( X^\dagger X \). It is simple to show that \( W \equiv UV^\dagger \) is the \( SU(N) \) matrix which maximizes \( \Re \text{Tr} X^\dagger W \). Unfortunately, \( \det UV^\dagger \neq 1 \).

2. Compute \( \det X \equiv \rho \exp(i\phi) \). The matrix \( \hat{X}_{NN} = \exp(-i\frac{\phi}{N})UV^\dagger \) is a suitable \( SU(N) \) matrix, adopted by Narayanan and Neuberger [16].

3. Find an approximate solution \( \{\theta_i\} \) for the phases of the diagonal matrix \( D = \text{diag}(\exp(i\theta_1),...\exp(i\theta_N)), \sum N \theta_i = 0 \mod 2\pi \), to maximize \( \Re \text{Tr} X^\dagger (\exp(-i\frac{\phi}{N})UDV^\dagger) \). To find an approximate solution to this non-linear problem, we assume that all phases \( \theta_i \) are small, and solve the linearized problem.

4. Accept the candidate \( U_{\text{new}} = \hat{X}U_{\text{old}}^\dagger \hat{X} \), where \( \hat{X} = \exp(-i\frac{\phi}{N})UDV^\dagger \), with probability Eq. (2) \(^5\).

### 2.2 Efficiency

We set out to compare the efficiency of the algorithm above with that of the standard \( SU(2) \) subgroup approach, as a function of \( N \). Going up to \( N = 10 \) forced us to

\(^5\) This corresponds to an overrelaxation parameter \( \omega = 2 \). It may be possible to make the algorithm more efficient by tuning \( \omega \), using the LHMC approach of [17].
consider a very small, $2^4$ system only. We chose a fixed 't Hooft coupling $g^2 N = 8/3$, so that $\beta = \frac{2N}{g^2} = \frac{3}{4} N^2$. This choice gives Wilson loop values varying smoothly with $N$, as shown in Fig. 2, and is representative of current $SU(N)$ studies. The Metropolis acceptance, as shown in Fig. 1, remains very close to 1. It increases with the 't Hooft coupling.

A first measure of efficiency is given by the average stepsize, i.e. the link change under each update. We measure this change simply by $\langle 1 - \frac{1}{N} \text{Re} \text{Tr} U_{\text{new}}^\dagger U_{\text{old}} \rangle$. The $SU(N)$ overrelaxation generates considerably larger steps than the $SU(2)$ subgroup approach, as visible in Fig. 3. The real test, of course, is the decorrelation of large Wilson loops. On our $2^4$ lattice, we cannot probe large distances. Polyakov loops (Fig. 4, left) show critical slowing down as $N$ increases, with a similar ex-
ponent $\sim 2.8$ using either update scheme. The $SU(N)$ strategy gives a speedup $O(3)$, more or less independent of $N$. One observable, however, indicates a different dependence on $N$ for the two algorithms. That is the asymmetry of the action, \[ \langle \sum x \operatorname{Re} \operatorname{Tr}(\text{Plaq}^\text{timelike} - \text{Plaq}^\text{spacelike}) \rangle. \] Fig. 4, right, shows that the speedup provided by the $SU(N)$ overrelaxation grows like $\sim N^{0.55}$. While this may be atypical, we never observed a slower decorrelation in the $SU(N)$ scheme for any observable.

In conclusion, overrelaxation in the full $SU(N)$ group appears superior to the standard $SU(2)$ subgroup approach. The results of [7] already indicated this for $SU(3)$. Our tests presented here suggest that the advantage grows with $N$, at least for some observables. For $SU(4)$ in $(2+1)$ dimensions [18], the decorrelation of the Polyakov loop was $\sim 3$ times faster in CPU time, using $SU(N)$ overrelaxation, although our code implementation used simple calls to LAPACK routines, which are not optimized for operations on $4 \times 4$ matrices. We definitely recommend $SU(N)$ overrelaxation for large-$N$ simulations.

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