SU(3) LATTICE GAUGE-FIXING
WITH OVER-RELAXATION AND GRIBOV COPIES

M.L. Paciello\(^1\), C. Parrinello\(^2\), S. Petrarca\(^3\), B. Taglienti\(^1\) and A. Vladikas\(^4\)

ABSTRACT

We report on the phenomenology of SU(3) lattice Landau type fixing as obtained by using an over-relaxation algorithm. An interesting result obtained using this very efficient algorithm is that distinct Gribov copies are generated by simply modifying the value \(\omega\) of the over-relaxation parameter for a fixed starting configuration.

By generating random gauge equivalent configurations, we study the variation of the number of copies with the lattice volume and gauge couplings.

\(^1\) INFN, Sezione di Roma La Sapienza, Piazzale A. Moro 2, I-00185 Roma.
\(^2\) Physics Department, New York University, 4 Washington Place, New York, NY 10003, U.S.A.
\(^3\) Theoretical Physics Division, CERN, CH-1211 Geneva 23 and INFN, Sezione di Roma, La Sapienza, Piazzale A. Moro 2, I-00185 Roma.
\(^4\) Dipartimento di Fisica, Università di Roma Tor Vergata, Via E. Carnevale, I-00173 Rome and INFN, Sezione di Roma Tor Vergata.

CERN-TH.6314/91
November 1991
In recent years, Monte Carlo simulations of lattice QCD involving gauge-dependent operators have become more important, both for technical reasons related to the adoption of smearing techniques [1],[2], and for the study of the (gauge-dependent) propagators of the fundamental fields entering the continuum QCD Lagrangian.

In fact, the study of gluon and quark propagators in some fixed gauge should provide insight into the relation between continuum and lattice models [3–6]. Moreover, quark and gluon matrix elements can be used to obtain renormalization conditions as proposed in [7].

The existence of Gribov copies [8–11] in the SU(3) lattice Landau and Coulomb gauges, which has been recently shown numerically for several different models [12–16], introduces conceptual difficulties, since the very definition of the lattice gauge becomes ambiguous and the numerical implementation of the gauge condition depends on the specific algorithm that is used.

On the other hand, it is not clear a priori whether all lattice Gribov copies are equivalent for the purpose of matching the result of a numerical gauge-dependent calculation with a continuum perturbative result, or whether one should ‘choose’ among the copies by imposing some additional constraint.

The standard way of fixing the Coulomb and Landau gauges on the lattice [17],[3],[18],[6] is based on the minimization of the quantity $F$:

$$F[U^g] \equiv -\frac{1}{V} \sum_n \sum_{k=1}^4 \text{Re} \, \text{Tr} \left( U_k^g(n) + U_k^g(n - \hat{k}) \right),$$

where $l$ is 3 for Coulomb and 4 for Landau gauge, $V$ is the lattice volume, $U_\mu(n)$ is a generic link, and by $U^g$ we mean the gauge-transformed link $U_\mu^g(n) \equiv g(n) U_\mu(n) g^\dagger(n + \hat{\mu})$. Once $F$ has been numerically minimized, the quantity $\theta$

$$\theta \equiv \frac{1}{V} \sum_n \theta(n) \equiv \frac{1}{V} \sum_n \text{Tr} \left[ \Delta^g(n) \Delta^g(n) \right],$$

where $\Delta^g(n) \equiv \sum_{k=1}^l \left( A_k^g(n) - A_k^g(n - \hat{k}) \right)$, is supposed to vanish, and this is the signal that the lattice gauge condition $\Delta(n) = 0$ is satisfied at each site. Actually in order to fix the gauge, i.e. in order to make (2) vanish, one just needs to reach any stationary point of $F$. The prescription of gauge-fixing to the minimum of $F$ was conjectured to be a good recipe for getting rid of possible lattice Gribov copies, in analogy to what was suggested by Gribov himself for the continuum model [8]. Unfortunately it has been shown to be insufficient for such a purpose [12–15]. An analogous problem has been shown to occur in the continuum [19], so that as far as the gauge-fixing problem is concerned, lattice gauge theories closely resemble the continuum ones, and this is of course very encouraging.

In this letter we employ the over-relaxation technique for gauge-fixing originally proposed by Mandula and Ogilvie [20]. For a general discussion on over-relaxation, see also refs. [21–26]. We will show that this kind of algorithm generates Gribov copies in an unconventional way.

This method consists of introducing a dependence of the gauge transformation field $r(n)$, which iteratively forces the link configurations towards the Landau gauge, on a real
parameter \( \omega \). This is done by replacing \( r(n) \) with \( r^\omega(n) \) and taking for \( r^\omega(n) \) a truncated binomial expansion:

\[
    r^\omega = \sum_{n=0}^{N} \frac{\gamma_n}{n!} (r - I)^n \quad \text{where} \quad \gamma_n = \frac{\Gamma(\omega + 1)}{\Gamma(\omega + 1 - n)}. \tag{3}
\]

In principle \( N \) in (3) should be infinite; in practice we have chosen \( N = 4 \) and verified that a similar phenomenon is obtained when taking \( N = 2 \). After the expansion, the new matrices \( r^\omega(n) \) are appropriately renormalized to \( SU(3) \). It is remarkable that the over-relaxation can be easily implemented to any algorithm for Landau or Coulomb gauge-fixing; the only change required is the expansion (3) at the end of each iteration of the normal gauge-fixing algorithm.

With this trick it is possible, on the lattices that we have considered, to gain typically a factor of between 3 and 5 in the number of iterations, while paying a computer time overhead of a factor of 1.5 for iteration, so that the resulting gain in time is at least a factor of 2.

Another small price to pay is related to the necessity of tuning \( \omega \) at an optimal value \( \omega_{\text{opt}} \), for which convergence is most rapid. This is done empirically, trying different values of \( \omega \); for our lattices we have found that \( \omega_{\text{opt}} \) does not depend on different configurations at fixed \( \beta \) and \( V \). For our \( \beta \) and \( V \) values it ranges between 1.70 and 1.75.

The standard way to study Gribov copies on the lattice consists of applying random gauge transformations on a thermalized link configuration \( U \); in such a way an ensemble of gauge-equivalent configurations is generated. Then all these configurations are gauge-fixed, and finally one checks whether the gauge-fixed configurations are all equivalent, i.e. related to each other by global gauge transformations, or not. In order to perform such a check, a good quantity to look at is the final value of \( F \), but of course there are other quantities [12] that can be utilized.

Our main result turns out to be that different choices for \( \omega \), besides influencing in a spectacular way the rate of convergence, may also lead to different Gribov copies when starting from the same initial configuration.

This can be qualitatively understood by recalling that non-linear dynamical systems (our gauge-fixing algorithm is equivalent to such a system) often exhibit a chaotic behaviour, in the sense that their evolution may depend dramatically both on the initial conditions (in our case this means different random initial gauge rotations) and on the relevant parameters of the evolution equations (the over-relaxation parameter \( \omega \)).

All the calculations have been performed for \( SU(3) \) lattices with Landau gauge-fixing, in double precision (64 bit), on an IBM RISC System/6000 mod 520 with 32 Mbyte of memory. Typically for \( V = 8^4 \) a single gauge-fixing sweep takes roughly 2 seconds.

In the figure we have shown the behaviour of \( \theta \) versus the number of gauge-fixing iterations for a lattice of \( V = 8^4 \) and \( \beta = 6 \). We have identified the curves corresponding to different copies giving the same letters \((\alpha, \beta, \gamma, \delta)\) to curves with the same final \( F \) value. As already observed in [20],[21],[22], it is possible to clearly distinguish two different regimes. The initial behaviour appears to be insensitive to the value of \( \omega \) and corresponds to large local fluctuations in the value of \( r(n) \) from one iteration to another. In the second regime, starting in our example after about 50 iterations, the fluctuations are smooth, characterized by a long range pattern; the rate of convergence is quite sensitive to the value of \( \omega \) since here one faces the problem of critical slowing down and the optimization of the algorithm becomes crucial. We are not able to say at which point the algorithm
takes different routes ending up with different copies, but as is shown in the figure, this happens frequently. Note that the behaviour of different curves is not directly related to the final value of $F$; moreover, the same final value of $F$ is sometimes obtained when using fairly different values of $\omega$.

Another quantity that can be monitored along the minimization sweeps is:

$$D[r] \equiv \frac{1}{V} \text{Tr} \sum_{n} \left( (r(n) - I)(r(n) - I)^{t} \right). \quad (4)$$

This measures the difference between the identity and the current gauge transformation along the gauge-fixing. An analogous quantity is used in ref. [14], without summing up the lattice points, to show for $SU(2)$ and $U(1)$ the distribution of this distance on the lattice for the gauge transformations relating different Gribov copies. Here we have studied $D[r]$ in order to see if this quantity has a different behaviour with respect to $\theta$, with the aim of gathering more information about the generation of different copies. We found that $D[r]$ manifests the same qualitative behaviour as $\theta$.

We remark that the fact that we find different copies for different values of a gauge-fixing parameter does not seem to give support to the idea [27] that prefixing the link configuration to some unambiguous gauge before Landau gauge-fixing would provide an unambiguous definition of the lattice Landau gauge.

We note that the Gribov copies obtained by starting from a fixed configuration and performing several gauge-fixing processes with different values of $\omega$, when regrouped according to the values of $F$, turn out to occur with the same relative frequencies as those generated by the usual procedure of applying random-starting gauge transformations.

We took advantage of the high efficiency of the over-relaxation technique in order to perform a preliminary study of the behaviour of Gribov copies with varying $\beta$ and lattice volume $V$. Using the standard method of starting random transformations, we have performed simulations in $SU(3)$ lattices with Landau gauge fixing for a number of $\beta$ and $V$ values as shown in the table. We have generated at least 3 thermalized configurations for each set of $(\beta, V)$ values; from each of these configurations, we have produced 21 random gauge-equivalent configurations and the Landau gauge has been fixed on each of them. The gauge-fixing is performed by reducing $\theta$ down to $10^{-18}$ and using the over-relaxation tuned at $\omega_{opt}$. The study of the number of copies as a function of the physical size has also been done for some cases in the deconfined phase [28].

Although the number of Gribov copies varies significantly from one thermalized configuration to another, our data show a tendency of the number of Gribov copies to decrease with shrinking physical lattice volume when the size of the physical box is varied by changing $V$ and $\beta$. This seems to be a general trend even if it is not observed at all points considered; see, for example, the point $(\beta, V) = (5.8, 8^4)$.

The decrease of the number of copies with decreasing physical lattice persists for $(\beta, V)$ values characteristic of the deconfined phase, but we point out that we still observe them across the phase transition for a few values of $\beta$. 
To summarize our work, we have pointed out that different minimization algorithms for $F$, even when applied to the same link configuration $U$, may converge to different Gribov copies. In addition we have presented a preliminary study of the occurrence of Gribov copies in the $SU(3)$ Landau gauge as a function of $(\beta, V)$. In connection with the latter point, a future more detailed analysis on larger lattices will enable us to investigate the possible relation between the (gauge-invariant) deconfinement transition and the decreased density of Gribov copies in the Landau gauge.

We thank G. Martinelli and M. Testa for their interest and encouragement, and G. Parisi and P. Rossi for discussions. A.V. acknowledges financial support from the EEC; C.P. acknowledges financial support from the CNR and S.P. would like to thank the CERN Theory Division for hospitality during this work.

REFERENCES


**Table:** The number of Gribov copies in $SU(3)$ lattices with varying $\beta$ and $V$; $L$ is the linear lattice size in GeV$^{-1}$ according to the two-loop perturbative asymptotic relation; $N_{\text{conf}}$ is the number of thermalized configurations generated in each case. The number of gauge-equivalent configurations fixed to the Landau gauge is always 21. Each entry stands for the number of copies found in each case: 1 stands for no copies found. The symbol (C) indicates the critical value of $\beta$; (*) stands for $\beta$ values characteristic of deconfinement.

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$L$ (GeV$^{-1}$)</th>
<th>$N_{\text{conf}}$</th>
<th>$V = 6^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.55</td>
<td>9.7</td>
<td>3</td>
<td>4, 1, 9</td>
</tr>
<tr>
<td>5.65</td>
<td>8.7</td>
<td>3</td>
<td>2, 4, 6</td>
</tr>
<tr>
<td>5.70</td>
<td>8.2</td>
<td>3</td>
<td>3, 2</td>
</tr>
<tr>
<td>6.00(*)</td>
<td>5.9</td>
<td>6</td>
<td>1, 1, 1, 1, 1, 4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$L$ (GeV$^{-1}$)</th>
<th>$N_{\text{conf}}$</th>
<th>$V = 8^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.65</td>
<td>11.6</td>
<td>3</td>
<td>9, 10, 4</td>
</tr>
<tr>
<td>5.80</td>
<td>9.8</td>
<td>6</td>
<td>1, 3, 1, 1, 7, 3, 1</td>
</tr>
<tr>
<td>6.00(C)</td>
<td>7.8</td>
<td>3</td>
<td>5, 6, 11</td>
</tr>
<tr>
<td>6.10(*)</td>
<td>7.0</td>
<td>3</td>
<td>2, 2, 2</td>
</tr>
<tr>
<td>6.20(*)</td>
<td>6.3</td>
<td>6</td>
<td>1, 1, 1, 2, 1, 1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$L$ (GeV$^{-1}$)</th>
<th>$N_{\text{conf}}$</th>
<th>$V = 10^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.65</td>
<td>14.5</td>
<td>3</td>
<td>12, 21, 3</td>
</tr>
</tbody>
</table>

**FIGURE CAPTION**

Plot of $\theta$ as a function of the Landau gauge-fixing sweeps for an $SU(3)$ lattice of $V = 8^4$ and $\beta = 6$. Different curves correspond to different $\omega$ values. The same letters ($\alpha, \beta, \gamma, \delta$) indicate curves with the same final $F$ value.