Abstract

We consider the design of a non-local Monte Carlo algorithm for $SU(3)$ lattice systems according to the idea of embedding the degrees of freedom corresponding to the center of the group $Z(3)$. As a crucial ingredient to reach this goal, we present a practical implementation of a cluster algorithm for $Z(3)$ systems with general random pair interaction.
I. Introduction

Developing non-local upgrade mechanisms for $SU(N)$ lattice models proved to be a rather hard task, because of the impossibility to carry on a straightforward generalization of Wolff’s embedding idea. There are apparently no such algorithms available for $SU(N)$ lattice systems, at present. The relatively small effort devoted to this goal has probably to do with the fact that the dynamics of gauge fields takes only a small part of the total computer time, and the feeling is that there is little to be gained in optimizing it. Still, large statistical errors on the gluon dynamics may result when large lattices will be used to explore more deeply the scaling region. We take the point of view that sometime it will pay to have an efficient algorithm for the pure gauge dynamics and we want to argue in this paper that a strategy similar to Brower-Tamayo’s embedding may possibly work, as suggested by Wolff. We present some preliminary steps to be taken to develop such an algorithm, even if their true value will be appreciated (hopefully) only after these ideas will be implemented in a realistic calculation. In order to simplify the presentation, we explicitly cover the $N=3$ two-dimensional sigma-model, but there seem to be no obstructions to generalize the idea to the case of four-dimensional QCD at finite temperature, which is the kind of real application we have in mind. According to ideas of Polyakov going back to the 70’s, it is precisely the center of the group which governs the deconfining transition, hence the $Z(3)$ degrees of freedom should be responsible for a critical slowing down near the critical temperature.

In sect. II we describe the simple embedding we have in mind for $SU(3)$; in sect. III we derive the algorithm and we give a few details on its implementation while in sect. IV we present some preliminary numerical results.

II. $Z(3)$ embedding

Embedding $Z(3)$ degrees of freedom into a $SU(3)$ model, like the non-linear sigma model, can be accomplished by assigning a cross section of the fibre bundle $Z(3) \rightarrow SU(3) \rightarrow SU(3)/Z(3)$. For instance such a section may be chosen as

$$ V \in SU(3) \rightarrow \zeta \cdot U \begin{cases} \zeta \in Z(3) \\ U \in SU(3)/Z(3) \end{cases} |\text{Arg} \{\text{Tr} U\}| < \pi/3 \quad (2.1) $$

Since the bundle is non-trivial, the section is only defined up to a set of measure zero, but this is fine for our purposes. The action transforms as follows (here and in the following $<ij>$ implies that $i$ and $j$ are nearest neighbours):  

$$ S = \sum_{<ij>} 4 \text{Re} \left\{ \text{Tr} V_i^\dagger V_j \right\} $$
\[ \sum_{\langle ij \rangle} \text{Re} \left\{ \bar{\zeta}_i \zeta_j \frac{1}{2} \text{Tr} U_i^\dagger U_j \right\} \]

and it appears as a $Z(3)$ model in the variables $\zeta$ with random couplings. In the gauge case, we would end up with a $Z(3)$ lattice gauge theory with random coupling. Near the continuum limit the matrix $U_i^\dagger U_j$ fluctuates around the identity, and the system is effectively ferromagnetic.

To exploit this embedding to beat critical slowing down at the continuum limit one needs an efficient algorithm for the $Z(3)$ degrees of freedom. While a cluster algorithm for $Z(3)$ spin systems is well-known in the real-constant-coupling case (a special case of $q$-Potts model with $q=3$), the random coupling case requires some modification. A general scheme for local pair interaction has been devised by Niedermayer and it covers the present situation. We are going to derive a cluster algorithm along a slightly different line of reasoning, but the outcome will be the same. Instead of concentrating on transition probabilities satisfying detailed balance, we shall introduce an equivalent ensemble with bond variables as new degrees of freedom, like one does in the Ising model. There are two ways to define the action in terms of bond variables and these correspond to two special cases in Niedermayer’s approach. The resulting cluster dynamics is non trivial in the first case while clusters are statistically independent in the second case.

III. The algorithm

Let us set the notation: $\zeta \in Z(3)$ is a generic spin variable, its values ranging on the set $(1, \omega, \bar{\omega})$, where $\omega = \exp(2\pi i/3)$. The action we consider is the following

\[ S = \sum_{\langle ij \rangle} \text{Re} \{ \bar{\zeta}_i \Omega_{ij} \zeta_j \} \]  

where $i, j$ range over pairs of next-neighbours.

The coupling constants $\Omega_{ij}$ are subject to a limitation which is not essential for the algorithm to work, but will simplify the presentation, namely we assume that

\[ |\text{Arg} \{ \Omega_{ij} \}| < \frac{2\pi}{3} \]  

for all $(i, j)$, a condition which is likely to be met near the continuum limit. Now let us write the partition function in the following way:

\[ Z = \prod_{\langle ij \rangle} Z_{ij} \]
\[ Z_{ij} = \exp(\beta \text{Re}\{\Omega_{ij}\})\delta_{\zeta_i, \zeta_j} + \exp(\beta \text{Re}\{\Omega_{ij}\bar{\omega}\})\delta_{\zeta_i, \omega\zeta_j} + \exp(\beta \text{Re}\{\Omega_{ij}\omega\})\delta_{\zeta_i, \bar{\omega}\zeta_j} \]

Ignoring a common factor \( \prod \exp(\beta \text{Re}\{\Omega_{ij}\}) \), we can rewrite \( Z \) as follows:

\[ Z = \prod_{<ij>} \left( \delta_{\zeta_i, \zeta_j} + W_{ij}(\bar{\omega})\delta_{\zeta_i, \omega\zeta_j} + W_{ij}(\omega)\delta_{\zeta_i, \bar{\omega}\zeta_j} \right) \quad (3.3) \]

where

\[ W_{ij}(z) = \exp(\beta \text{Re}\{(z - 1)\Omega_{ij}\}) \]

On each link \( ij \) let us define

\[ W_{ij}^< = \min(W_{ij}(\omega), W_{ij}(\bar{\omega})) \]
\[ W_{ij}^> = \max(W_{ij}(\omega), W_{ij}(\bar{\omega})) \quad (3.4) \]

and

\[ \omega_{ij}^b = \begin{cases} \omega & \text{if } W_{ij}^> = W(\omega) \\ \bar{\omega} & \text{otherwise} \end{cases} \quad (3.5) \]

Under the condition above on the phase of \( \Omega \) (Eq. 3.2), it turns out that \( W^< < 1 \); as a consequence, if we rewrite \( Z_{ij} \) as follows:

\[ Z_{ij} = \delta_{\zeta_i, \zeta_j} + W_{ij}^<(1 - \delta_{\zeta_i, \zeta_j}) + (W_{ij}^> - W_{ij}^<)\delta_{\zeta_i, \omega\zeta_j} \quad (3.6) \]

we can introduce bond variables \( n_{ij} \) as in Swendsen-Wang's algorithm, to get either

\[ Z = \sum_{\zeta, n} \prod_{<ij>} \left\{ \delta_{n_{ij}, 1}\delta_{\zeta_i, \zeta_j}(1 - W_{ij}^<) + \delta_{n_{ij}, 0}[W_{ij}^< + (W_{ij}^> - W_{ij}^<)\delta_{\zeta_i, \omega\zeta_j}] \right\} \quad (3.7) \]

or

\[ Z = \sum_{\zeta, n} \prod_{<ij>} \left\{ \delta_{n_{ij}, 1}[\delta_{\zeta_i, \zeta_j}(1 - W_{ij}^<) + \delta_{\zeta_i, \omega\zeta_j}(W_{ij}^> - W_{ij}^<))] + \delta_{n_{ij}, 0}W_{ij}^< \right\} \quad (3.8) \]

As a first option we then have the following updating algorithm: first step, the bonds are switched on with probability \( (1 - W_{ij}^<) \), provided \( \zeta_i = \zeta_j \) (this first step is identical to Swendsen-Wang's). The second step is given by the spin update, which is governed by the term \( \delta_{n_{ij}, 1} \), forcing the same spin value on each connected cluster. These cluster spin values are chosen according to a distribution \( Z_{\text{clust}} \) which takes into account cluster interaction which occurs at the boundaries. The effective action for the cluster dynamics can be extracted from the term involving \( \delta_{n_{ij}, 0} \). Let \( C \) denote a generic cluster, \( \zeta_C \) its spin; then we have

\[ Z_{\text{clust}} = \prod_{C, \bar{C}} W(\zeta_C, \bar{C'}) \]
where
\[
W(\zeta_C, \zeta_C') = \prod_{<ij>} \left( W_{ij}^\geq + (W_{ij}^\leq - W_{ij}^\geq) \delta_{\zeta_C, \omega_{ij}^\flat \zeta_C'} \right)
\]

The clusters’ interaction dictated by this formula can be now treated as an ordinary lattice system, e.g. by a heat bath method. What we have realized here is a transformation from the original \(Z(3)\) lattice system to another \(Z(3)\) system indexed by clusters. The implementation which we have already tested (see next section) is suggested by Wolff’s single cluster algorithm. The assumption underlying such a choice is that in some equilibrium regime the existing spin values on the boundary of the cluster can be used to evaluate the probability distribution even without growing the other clusters.

As for the second option, starting from Eq. 3.8 the bonds are switched on with probability
\[
\begin{cases}
1 - W^\leq & \text{if } \zeta_i = \zeta_j \\
1 - W^\geq & \text{if } \zeta_i = \omega_{ij}^\flat \zeta_j \\
0 & \text{otherwise}
\end{cases}
\]

There is no interaction between clusters (which may be read from the fact that the coefficient \(\delta_{n,0}\) is \(\zeta\)-independent), but the interaction among spins within a cluster is non trivial. Instead of trying to thermalize the system on each cluster, we can just apply a global rotation chosen independently at random on each cluster. Niedermayer showed that this move satisfies detailed balance and ergodicity is obviously satisfied since clusters with just one site are possible.

The setup outlined here would not work in case Eq. 3.2 is violated somewhere. It is however straightforward to modify the formulae to account for this.

IV. Preliminary numerical results

We have implemented the first option (single cluster) to simulate a two-dimensional \(Z(3)\) model with random coupling. The coupling \(\Omega_{ij}\) is uniformly distributed in the region
\[
\left( \frac{1}{2} < \text{Re} \{ \Omega \} < \frac{3}{2} \right) \cap \left( |\text{Arg} \{ \Omega \}| < \pi/3 \right).
\]

In order to count sweeps in a fair way, we defined a sweep as consisting of an update on \(\Omega\) followed by \(N_{\text{hits}}\) cluster updates, with \(N_{\text{hits}}\) adaptively chosen in such a way that \(N_{\text{hits}} \times < N_c > \approx L^2\), where \(< N_c >\) is the average cluster size and \(L\) is the lattice size. In this way the computer time for a sweep is essentially independent on \(\beta\). The autocorrelation time \(\tau_{\text{int}}\) has been measured for the total magnetization \(< \zeta >\) using the formula given in [4]. We report the correlation length \(\xi\) for \(< \text{Re} \{ \zeta_i \zeta_j \} >\) projected at vanishing transverse momentum, together with \(\tau_{\text{int}}\) and the average linear size of the clusters. Data have been
taken on a 128 × 128 lattice on several runs of 5000 sweeps each (Tab.1) and on a 200 × 200 lattice with 2500 sweeps only (Tab.2).

The numerical data show a clear sign of critical behaviour around $\beta \approx 0.615$. At the same time the autocorrelation time $\tau_{int}$ does not increase more than linearly in $\xi$, at least up to $\beta \approx 0.610$; beyond this value $\xi$ becomes a substantial fraction of the lattice size and $\tau_{int}$ starts to grow more rapidly. To determine the dynamic critical exponent for the algorithm one needs a very high statistics, and our data are too preliminary to get a reliable conclusion. The sharp rise in $\tau_{int}$ near the transition, if confirmed, would mean that the algorithm is not as efficient as we would have expected, but it may still be of some practical value – since the actual values are not dramatically high. One also remarks that going to bigger lattices tends to improve the performance.

V. Conclusions

We have examined the feasibility of a cluster algorithm designed to embed $Z(3)$ into $SU(3)$ in the spirit of Brower and Tamayo. Clearly most of the work is still to be done. We have to combine the present $Z(3)$ algorithm with some local update mechanism for the $SU(3)/Z(3)$ degrees of freedom. This should carefully deal with the coset condition 2.1 – a heat bath technique would probably be best suited. For the application to gauge theory one has to further modify the algorithm, but some progress was done recently on gauge $Z(2)$ and $U(1)$ systems, and also this problem will hopefully be overcome.

What will the overhead be for such kind of algorithm, say in the study of the deconfining transition? Judging from recent progress in implementing cluster algorithms on massively parallel machines[6][7], the price to be paid should not be too high.

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### Table 1: 128 × 128

| $\beta$ | $\xi$ | $\tau_{int}$ | $\sqrt{<N_c>}$ |
|---------|-------|--------------|-----------------|
| .560    | 2.3   | 1.0          | 4               |
| .580    | 3.0   | 1.0          | 5               |
| .600    | 4.7   | 1.2          | 8               |
| .602    | 5.2   | 1.3          | 8               |
| .604    | 5.7   | 1.3          | 9               |
| .606    | 6.3   | 1.4          | 10              |
| .608    | 7.7   | 1.9          | 11              |
| .610    | 12.0  | 3.5          | 16              |
| .612    | $\approx 25$ | $\approx 22$ | $32$            |

### Table 2: 200 × 200

| $\beta$ | $\xi$ | $\tau_{int}$ | $\sqrt{<N_c>}$ |
|---------|-------|--------------|-----------------|
| .600    | 4.7   | 1.0          | 7               |
| .602    | 4.9   | 1.2          | 8               |
| .604    | 5.5   | 1.3          | 9               |
| .606    | 6.2   | 1.5          | 10              |
| .608    | 7.6   | 1.6          | 11              |
| .610    | 9.3   | 2.5          | 14              |
| .612    | 18.0  | 12.0         | 23              |
| .613    | $\approx 25$ | $\approx 21$ | $33$            |
| .614    | $\approx 32$ | $\approx 40$ | $41$            |