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TOWARDS CLUSTER ALGORITHMS FOR SU(2) GAUGE THEORIES

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We present a cluster algorithm for the $N_t = 1$ finite temperature SU(2) gauge theory. The algorithm efficiently flips the signs of the Polyakov loops; ergodicity is ensured by combining it with a standard local procedure. The dependence of the autocorrelation time on the ratio between the number of cluster steps and that of local steps is investigated in detail. At the finite temperature transition, critical slowing down is reduced drastically, the dynamical critical exponent z for the combined algorithm being $z \simeq 0.5$.

Finding an efficient simulation algorithm for pure gauge theories is one of the main challenges in lattice gauge theories. In this paper we report on a new cluster algorithm for the finite temperature SU(2) pure gauge theory in $3+1$ dimensions, which is defined by the action

$$S = -\beta \sum_p \tfrac{1}{2} \mathrm{Tr} U(p) . \qquad (1)$$

Here $U_{x,\mu}$ are 2×2 SU(2) matrices, x is a site on an $L^3 \times N_t$ lattice, x,μ is a link of this lattice, and $U(p)$ is the product of link variables along the boundary of an elementary plaquette p. Periodic boundary conditions are assumed.

One of the main guiding principles in devising efficient algorithms is to try to act directly on the relevant degrees of freedom. At least for small N_t, it is accepted by now[1] that these are the Polyakov loops $P_{\underline{x}}$,

$$P_{\underline{x}} := \tfrac{1}{2} \mathrm{Tr} \prod_{t=1}^{N_t} U_{(\underline{x},t),0} . \qquad (2)$$

Here the underlined quantities denote spatial objects (3 dimensions), and $(\underline{x},t)$ is the 3+1 dimensional notation for a 4-dimensional point.

We attempted to devise *cluster algorithms* (see e.g. [2, 3, 4]) that significantly speed up the Polyakov loop pseudodynamics. As the basis for such algorithms we used a representation in which the *embedded Ising variables*[5, 3, 4] are the signs of the Polyakov loops. The clusters are built using the effective interaction for these variables, and "flipped" by changing their signs. In order to ensure ergodicity, the cluster updates have to be supplemented by conventional local upates.

One way to have the Polyakov loops among the degrees of freedom in terms of which the model is written is to go to the temporal gauge ("$A_0 = 0$"). Now, in order to obtain a successful algorithm, that does overcome critical slowing down, the embedded Ising model should not be frustrated[2, 3, 4]. For the signs of the Polyakov loops however, we get an effective interaction that is frustrated. Furthermore, we also get an undesired magnetic field term, whose fluctuating sign and strength depends on the other degrees of freedom.

For the case of $N_t = 1$ an important simplification occurs: there is no frustration and no magnetic field term. For the timelike plaquette p that connects the spatial points $\underline{x}$ and $\underline{x} + \hat{j}$ ($\hat{j}$ is a lattice spacing vector in the spatial j-direction),

$$\tfrac{1}{2} \mathrm{Tr} U(p) = P_{\underline{x}} P_{\underline{x}+\hat{j}} + \text{const.} , \qquad (3)$$

where the constant does not depend on the signs of $P_{\underline{x}}$ and $P_{\underline{x}+\hat{j}}$. This corresponds to a ferromagnetic interaction of the embedded Ising variables, the effective coupling being $\beta |P_{\underline{x}} P_{\underline{x}+\hat{j}}|$.

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In this situation our cluster algorithm is defined as follows. First we delete or freeze the links $\underline{x}, j$ (we use here the terminology of [6]). The deletion probability for a link is

$$P_{del}(\underline{x}, j) = \exp\left\{-\beta\left(P_{\underline{x}}P_{\underline{x}+j} + |P_{\underline{x}}P_{\underline{x}+j}|\right)\right\} . \quad (4)$$

The freezing probability is $1 - P_{del}(\underline{x}, j)$. Two sites are connected if they are at the endpoints of a frozen link. A cluster is a connected set of sites (all links from a site in the cluster to one outside it are deleted). In order to update the configuration we use the single-cluster algorithm[3]: a cluster is "grown" around a randomly chosen site (the seed) and flipped with probability one. This achieves a flip $P_{\underline{x}} \to -P_{\underline{x}}$ for the Polyakov loops in the cluster.

We supplemented the cluster update with a local update of all degrees of freedom. For the timelike links we used the heath bath procedure of [8]. Because of the $N_t = 1$ condition, we had to use a Metropolis procedure to update the spatial links.

Although the $N_t = 1$ case is not really the physically relevant one, we decided to study it in detail for a variety of reasons:

- It is a test of whether our whole approach for obtaining a cluster algorithm for the study of the finite temperature transition is meaningful. It is not a priori clear that speeding up the Polyakov loop updates alone will suffice to overcome critical slowing down.
- There is little experience in the analysis of the autocorrelations in a situation where a nonergodic cluster algorithm is combined with an ergodic local algorithm.
- At the present stage, any progress at all in cluster algorithms for gauge theories may be relevant.

Even for $N_t = 1$, a careful measurement of the dynamical critical exponent z[7, 2, 3, 4] was a very CPU intensive study, because we still had to deal with a 3 dimensional $SU(2)$ system and with an a priori arbitrary mixture of 2 algorithms (cluster and local).

We first determined the exact location of the phase transition from a standard finite size analysis. We obtained $\beta_c = 0.8730(2)$ and critical exponents

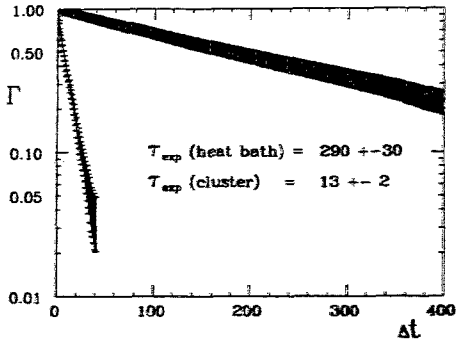

Figure 1: Autocorrelation functions for Polyakov loops $\bar{L}$ on a $32^3 \times 1$ lattice at the phase transition *with* ($R = 0.18$) and *without* clusters.

compatible with those of the three-dimensional Ising model. We shall not give details of this analysis here, since, up to the exact location of β_c, the results are exactly what we expected.

Let us define one time unit in the Markov chain we generate during the simulation as one local sweep followed by n cluster flips. In order to determine z, we go to the critical point and check the relation[7, 2, 3, 4] $\tau \propto L^z$, where τ is the *exponential* autocorrelation time (i.e. the *slowest* mode of the update procedure)[4]. We compare runs at different values of L for which the ratio R,

$$R := n\,\frac{\langle \text{clustersize} \rangle}{L^3}, \quad (5)$$

of the work performed in the cluster part to that performed in the local part is constant. Studying the dependence of τ on R is also very interesting, since little is known about the analysis of critical slowing down for a mixed algorithm. Notice that the limit $R \to \infty$ is the "idealized embedding" discussed in [4].

For a sufficiently accurate determination of τ, the runs at β_c were very long, between 30000 and 100000 time units (for the study of the critical properties alone, much shorter runs suffice, since our algorithm is very efficient). We measured a large number of observables, including space- and timelike plaquettes, absolute value of the lattice-averaged Polyakov loop $\bar{L} := \left|\frac{1}{L^3}\sum_{\underline{x}} P_{\underline{x}}\right|$, etc.. We also defined and measured *improved observables*[3], e.g.

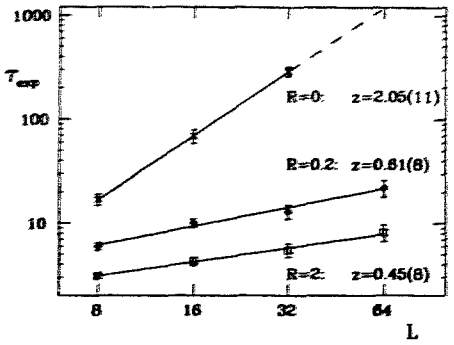

Figure 2: Autocorrelation times versus lattice size for zero, few and many cluster updates per sweep (from autocorrelations of Polyakov loops).

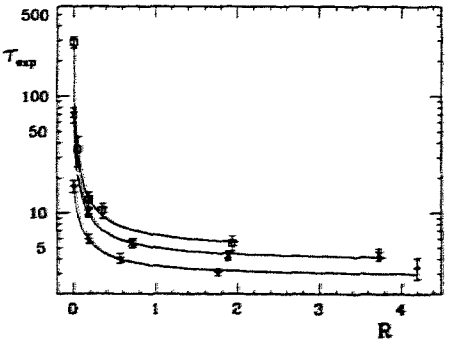

Figure 3: Autocorrelation times versus R for lattice sizes $L = 8, 16, 32$. The curves are fits according to (6).

for correlations between Polyakov loops. Exponential autocorrelation times for *all* observables that did show slowing down at all were consistent (there were no visible autocorrelations in spacelike plaquettes).

We took great care to perform a thorough error analysis. We took into account the covariances of autocorrelations at different time distances. We checked all results for stability with a complete Jackknife analysis. We were also careful to verify that the plots of the autocorrelation functions do show a clear exponential decay – such a check had turned out to be crucial during a concurrent cluster investigation[9].

Let us now turn to the description of our results concerning the performance of our algorithm. First and utmost, the new algorithm spectacularly reduces critical slowing down. To exemplify this, we compare in fig.1 two autocorrelation functions for a $32^3 \times 1$ lattice at $\beta = 0.8730$, one for a purely local update, the other for $R = 0.18$ (i.e. per local sweep, only 18% of the lattice sites are changed by cluster updates). Yet the speedup is tremendous! The $64^3 \times 1$ lattice would have been totally unaccessible without cluster updates.

For two quite different values of R, we performed measurements of z (only the $L = 64$ runs were really expensive; for smaller values of L we also took other R's – see below). Within statistical errors, the relation $\tau \propto L^z$ was well obeyed, as seen from fig. 2. We obtained $z = 2.05(11)$ for the purely local update (as expected), which was drastically reduced by the inclusion of clusters to $z = 0.61(8)$ for $R \simeq 0.2$ and $z = 0.45(8)$ for $R \simeq 2$!

It is remarkable that the value of z stabilizes at small values of R already. In order to further study the R-dependence of the autocorrelation time, we performed additional runs for $L = 8$, 16 and 32. The results are presented in fig. 3. $\tau(R)$ at fixed L shows a very fast initial dropoff, roughly like $1/R$. It goes to a constant asymptotic value τ_∞ as $R \to \infty$, which corresponds to the "idealized algorithm" of [4]. Fig. 3 suggests that $R = 2$ is almost asymptotic already!

In our implementation, CPU time is proportional to $(1 + R)$, and $R \approx 0.5$ will be the most effective algorithm (in our case the local part vectorized completely; otherwise a larger value of R would give optimal performance).

It is amusing to note that the results of fig. 3 are well described by

$$\tau = \tau_\infty + \frac{\tau_{cl}}{R + \epsilon}; \qquad (6)$$

where τ_∞ is the autocorrelation time of the idealized ($R \to \infty$) algorithm, τ_{cl} (≈ 1) may be interpreted as the autocorrelation time for cluster updates of the effective Ising models, and the small quantity ϵ corresponds to the large autocorrelation time of the purely local algorithm.

The small values of τ_{cl} and of τ_{∞} suggest that the cluster update is almost perfect in the space of the embedded Ising variables, whereas the local update is very good in the space of all other degrees of freedom (but very bad at flipping the Polyakov loops).

Thus we have shown, for the first time ever in the framework of lattice gauge theories, that cluster updates of the proper physical degrees of freedom can strongly reduce critical slowing down, even when they have to be combined with local updates for the other degrees of freedom. A more detailed account of this investigation will be published elsewhere.

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