Tests of globally corrected hybrid updating

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We test globally corrected hybrid updating algorithms for various lattice theories: a chain of coupled harmonic oscillators, pure SU(3) theory, and QCD with four flavors of dynamical staggered quarks. Systematic errors, acceptance, and time correlations are studied as functions of discretization step size, momentum refreshing frequency, volume, coupling and fermion-matrix-inversion residue.

I. INTRODUCTION

The lack of algorithms which are both exact and efficient is the major obstacle on the road towards truly realistic supercomputer simulations of QCD with light dynamical quarks.

Updating algorithms such as pseudofermions,[1] Langevin[2] or hybrid dynamics[3] allow, at the price of many hundred CPU hours on a present-generation supercomputer, hadron mass calculations on lattices up to $10^3\times 32$, for quark masses as low as 0.025 (in lattice units) and for β as large as 5.7 ($\beta=6/g^2$, where g is the QCD coupling).[4] In the exploration of the phase structure of finite-temperature QCD, the corresponding "world records" are $10^3\times 6$ lattices and quark mass 0.0125 in lattice units.[4] However, each of these algorithms relies on some approximation which makes them violate detailed balance as they explore phase space with a finite step size. At best, the resulting systematic errors can be computed analytically to second order in the step size.[2,3,5] Therefore, the results of these expensive supercomputations are subject to some bias which is not precisely known; in addition, it is not rigorously possible to compare results obtained by different algorithms. Efficient algorithms which do not make use of such approximations would be required to establish high-statistics benchmarks by which to judge the performance of various approximate algorithms.[5] If they were efficient enough, exact updating algorithms could even be used for production runs.

The reason why relatively large lattices are affordable with the approximate algorithms is that the computer time required for a given number of sweeps through the lattice grows only proportionally to the lattice volume. By contrast, a naive direct evaluation of the fermion determinant implies a volume-to-the-fourth-power computer time dependence. Various schemes have been proposed in order to obtain a less disastrous growth, while maintaining detailed balance.[6-10] The algorithms which obey detailed balance locally[6,7] can achieve at best a volume-squared increase in computer time.[10] The algorithms which combine Langevin or hybrid updating with a global accept/reject step at the end of the lattice sweep[8-10] promise to yield a more favorable volume dependence.[10]

In practice, one would like such an exact algorithm to allow larger step sizes than those permitted by approximate updating methods. Then, the increased cost of updating would be offset by the more efficient exploration of phase space. However, large changes might cause low acceptance probabilities of the proposed new configurations, so that the evolution would be actually slowed down. The same effect might appear due to an increase in volume or in the length of the molecular-dynamics trajectories. Too low or too high an acceptance rate might mean large correlations between configurations. The interdependences of these various parameters could be strongly affected by changes in the gauge coupling and in the fermion mass. There is the additional question of the influence of the accuracy with which the fermion matrix is inverted.

We have addressed some of these problems for various systems with and without fermions. We have compared the systematic errors of uncorrected and globally corrected hybrid updating as a function of the step size for various couplings. We have studied the dependence of the acceptance and of the correlation between configurations on the step size, on the number of degrees of freedom, and on the length of the trajectory. For full QCD, we have also tested the dependence of the acceptance upon the conjugate-gradient inversion residue.

The algorithms we use are presented in Sec. II. Section III contains our numerical results for a linear system of coupled harmonic oscillators. Results for pure SU(3) theory are given in Sec. IV and those for QCD appear in Sec. V. Some conclusions are offered in Sec. VI.

II. GLOBALLY CORRECTED HYBRID UPDATING

Consider a linear chain of N coupled harmonic oscillators. The action is

$$S=\sum_i(-x_{i+1}x_i+\mu x_i^2)\ . \tag{1}$$

In this notation, the critical coupling of the model is $\mu=1$. To simulate this system numerically, one generates a Markov chain of configurations $\{x\},\{x'\},\ldots$. The probability for the transition to a new configuration $P(\{x'\}\,|\,\{x\})$ must satisfy the detailed-balance condition

$$P(\{x'\}\,|\,\{x\})P(\{x\})=P(\{x\}\,|\,\{x'\})P(\{x'\})\ , \tag{2}$$

where $P(\{x\})=C\exp[-S(\{x\})]$. A classic paper[11] established that this condition can be implemented by proposing some trial change in the configuration and accepting it with the conditional probability

$$P_{\rm acc}=\min\left[1,\frac{P_T(\{x\}\mid\{x'\})P(\{x'\})}{P_T(\{x'\}\mid\{x\})P(\{x\})}\right], \tag{3}$$

where $P_T(\{x'\}\mid\{x\})$ is the probability of selecting a trial configuration $\{x'\}$ starting from configuration $\{x\}$.

Let us choose the following global trial change:

$$x_i'=x_i-\frac{\partial S(\{x\})}{\partial x_i}\frac{\delta t^2}{2}+p_i\delta t \tag{4}$$

for all sites $i=1,N$, where the p_i are standard Gaussian noise with unit variance and zero mean. δt is a parameter which describes the magnitude of the change. The corresponding global trial probability $P_T(\{x'\}\mid\{x\})$ is proportional to $\exp(-\sum_i p_i^2/2)$. The reverse trial probability (to obtain $\{x\}$ from $\{x'\}$) is proportional to $\exp(-\sum_i p_i'^2/2)$ with

$$p_i'=p_i-\left[\frac{\partial S(\{x\})}{\partial x_i}+\frac{\partial S(\{x'\})}{\partial x_i'}\right]\frac{\delta t}{2}. \tag{5}$$

Substituting into Eq. (3) yields

$$P_{\rm acc}=\min\left[1,\frac{\exp[-H(\{x'\},\{p'\})]}{\exp[-H(\{x\},\{p\})]}\right] \tag{6}$$

with the notation $H=\sum_i p_i^2/2+S(\{x\})$.

This notation is not accidental: Eqs. (4) and (5) are in fact a reversible, area-preserving discretization scheme for the Hamiltonian evolution of the system in phase space, as a function of the time variable t. H is the system Hamiltonian and the p_i are the canonical momenta conjugate to the x_i:

$$dx_i=p_i dt\ ,\quad dp_i=-\frac{\partial H(\{x\},\{p\})}{\partial x_i}dt=-\frac{\partial S(\{x\})}{\partial x_i}dt\ . \tag{7}$$

The so-called "leap-frog" discretization of these differential equations proceeds as follows:[9]

$$p_i(\delta t/2)=p_i(0)-\left.\frac{\partial S}{\partial x_i}\right|_{t=0}\frac{\delta t}{2} \tag{8}$$

is the initial half-step; this is followed by $n=t'/\delta t$ steps for x_i and $n-1$ steps for p_i:

$$x_i(t+\delta t)=x_i(t)+p_i(t+\delta t/2)\delta t\ , \tag{9}$$

$$p_i(t+\delta t/2)=p_i(t-\delta t/2)-\left.\frac{\partial S}{\partial x_i}\right|_t\delta t\ ; \tag{10}$$

and finally by a last half-step for p_i:

$$p_i(t')=p(t'-\delta t/2)-\left.\frac{\partial S}{\partial x_i}\right|_{t=t'}\frac{\delta t}{2}\ . \tag{11}$$

Since Eqs. (8)–(11) can be rewritten in the form of Eqs. (4) and (5) by setting $x_i'=x_i(t')$ and $p_i'=p_i(t')$, these two discretizations are identical and either form can be implemented numerically.[9,10]

Such an implementation begins with a random momentum configuration $\{p(0)\}$ and with the computation of the initial value of the Hamiltonian. After completing n deterministic steps according to Eqs. (4) and (5) or (8)–(11), one obtains a final trial configuration which is subjected to an accept/reject step according to Eq. (6). The whole procedure is then repeated until the desired number of configurations has been generated. The initial choice of momenta and the n deterministic steps define a trajectory through phase space. In the limit $\delta t\to 0$ this trajectory becomes microcanonical ($\delta H=0$). For $n=1$, the procedure reduces to the simple Euler discretization of the system's Langevin equation. When $n>1$, it is a hybrid updating algorithm.[3]

Now consider the case of a theory whose variables U are elements of an unitary group with generators T^α which satisfy $\mathrm{tr}(T^\alpha T^\beta)=\delta_{\alpha\beta}/2$. Its Hamiltonian will be

$$H=\sum_i \mathrm{tr}(p_i^2)+S(\{U\})\ . \tag{12}$$

The canonical momenta p_i are elements of the algebra ($p_i=\eta_i^\alpha T^\alpha$). The Hamilton equations for this system read

$$dp_i=-\nabla_i^\alpha S(\{U\})T^\alpha dt\ ,\quad dU_i=iU_i p_i dt\ . \tag{13}$$

(∇_i^α is the group-invariant derivative.) The globally corrected hybrid algorithm can be applied to the discretized form of these equations. We have tested the algorithm for pure SU(3) theory with the Wilson action:

$$S_G=-\beta\sum_{\square}(\mathrm{tr}U_{\square}+\mathrm{tr}U_{\square}^\dagger)\ . \tag{14}$$

The corresponding effective action for full QCD with n_f flavors of staggered quarks is

$$S=S_G-\frac{n_f}{4}\mathrm{tr}\ln(M^\dagger M)\ , \tag{15}$$

where $M(\{U\})$ is the lattice Dirac operator; $M^\dagger M$ is only defined on even lattice sites, thus avoiding an additional species doubling.[12] For this system, Eqs. (4) and (5) become

$$U_i'=U_i\exp\left[i\left[F_i^\alpha(\{U\},\{\chi\})T^\alpha\frac{\delta t^2}{2}+p_i\delta t\right]\right], \tag{16}$$

$$p_i'=p_i+[F_i^\alpha(\{U\},\{\chi\})+F_i^\alpha(\{U'\},\{\chi'\})]T^\alpha\frac{\delta t}{2}\ . \tag{17}$$

F_i^α is the driving force:

$$F_i^\alpha=-\nabla_i^\alpha S_G+\frac{n_f}{4}\chi^\dagger M^{\dagger-1}\nabla_i^\alpha(M^\dagger M)M^{-1}\chi\ , \tag{18}$$

where the Gaussian noise χ (with unit variance) serves to estimate the group-invariant derivative of the fermionic part of the action.[2,5] In Eqs. (16)–(18), the index i runs over all links.

Equations (16) and (17) still obey the reversibility requirement which is necessary for detailed balance. As shown for instance in Ref. 10, detailed balance can be enforced in this case by accepting the new configuration with the probability

$$P_{\rm acc}=\min\left[1,\frac{\exp\left[-\sum_i \mathrm{tr}(p_i'^2)\right]e^{-S_G(\{U'\})}e^{-\phi^\dagger(M'^\dagger M')^{-1}\phi}}{\exp\left[-\sum_i \mathrm{tr}(p_i^2)\right]e^{-S_G(\{U\})}e^{-\phi^\dagger(M^\dagger M)^{-1}\phi}}\right]. \tag{19}$$

We use the notation $M'=M(\{U'\})$. ϕ are pseudofermionic fields updated by the heatbath procedure $\phi=M^\dagger\xi$ (the ξ's are another set of Gaussian random numbers with unit variance).

From the computational point of view, the problem with simulating Eqs. (16) and (17) is that the matrix exponentiation in (16) should be done exactly. Otherwise reversibility and Liouville's thereom will be violated. In practice, one usually keeps a number k of terms in the series expansion of the matrix exponential. Such a procedure must always be followed by an explicit reunitarization, which ensures that the new U's are group elements. This still violates detailed balance to order $k+1$ in the step size. The importance of this residual source of systematic errors in the globally corrected algorithm can be tested by comparing the results to some exact algorithm (see Sec. IV).

Whereas the evolution equations (16)–(18) are valid for any n_f, the acceptance criterion (19) allows only multiples of $n_f=4$, otherwise detailed balance is violated. The globally corrected hybrid algorithm for full QCD which we have described above is a variation of those introduced in Refs. 9 and 10, because we use the noisy estimator method[5] during the n molecular-dynamics steps. We believe it is worthwhile to test this method because it is known to be faster in uncorrected Langevin and hybrid updating. As we pointed out above, the process still satisfies detailed balance. However, the final Hamiltonian is no longer a deterministic function of the initial state. In the limit of vanishing step size, the evolution is microcanonical with probability 1 with respect to the noisy estimator sample: $\langle \delta H\rangle_{\{\chi\}}\to 0$ for $\delta t\to 0$. There might be a loss of acceptance with respect to the deterministic evolution for small volumes, but this effect should decrease with increasing lattice volume.

III. A CHAIN OF COUPLED HARMONIC OSCILLATORS

Our first task is to verify that the globally corrected algorithm is indeed exact for any step size δt. This is easily done for the case of the simple system (1). The quantity $\langle x^2\rangle$ can be computed exactly for a given chain length (lattice volume) N and for a given coupling μ. We have determined that the exact result becomes almost independent of the volume for $N\geq 100$. With the notation of Eq. (1), the critical coupling of the model is $\mu=1$.

We have applied the globally corrected as well as the uncorrected hybrid algorithm for $N=100$ oscillators with several values of μ. Figure 1 compares the results of up to 5×10^5 lattice sweeps to the known exact values of $\langle x^2\rangle$. Figure 1(a) shows that the uncorrected algorithm starts deviating markedly from the exact result for $\delta t\geq 0.25$. By contrast, the corrected algorithm continues

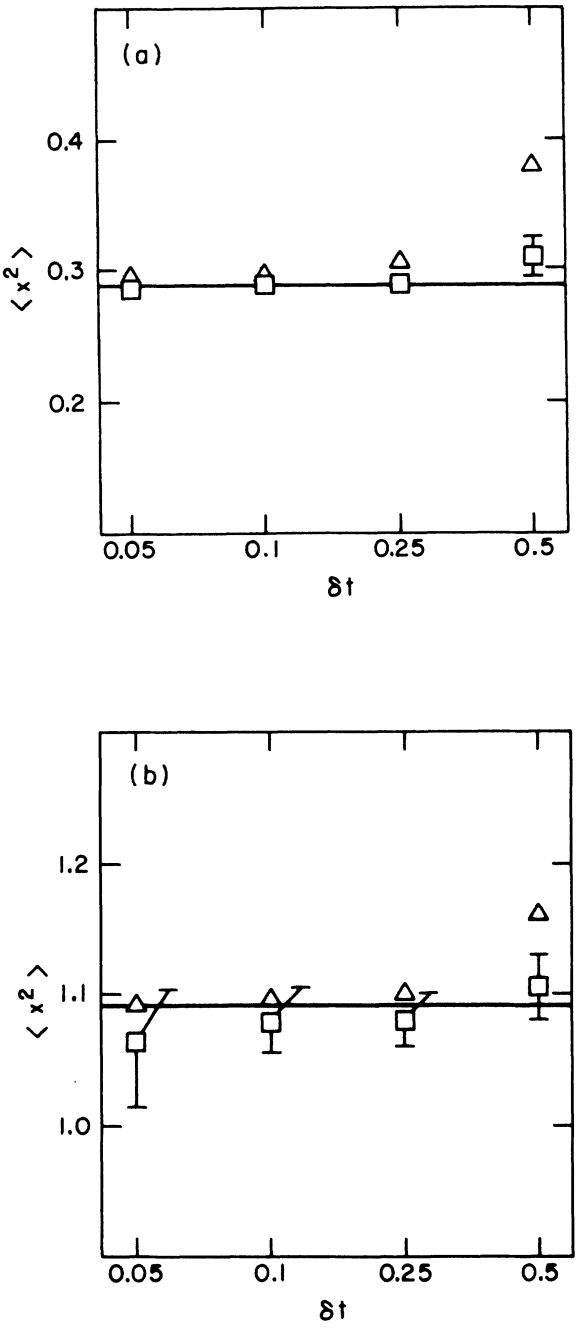

FIG. 1. Accuracy of globally corrected and of uncorrected hybrid updating for a chain of $N=100$ coupled harmonic oscillators. The straight lines are results of exact computations. Squares denote the results of corrected Langevin updating ($n=1$ molecular-dynamics step) and triangles represent the results of uncorrected hybrid updating ($n=5$ molecular-dynamics steps). (a) is for $\mu=2$ and (b) is for $\mu=1.1$.

to reproduce the exact result. The same qualitative results were obtained for lower μ [see Fig. 1(b) for $\mu=1.1$]. The error bars become larger when we approach criticality, but within statistics the corrected algorithm remains exact for all investigated step sizes and couplings.

Figure 2 shows the dependence of the acceptance rate and of the correlation between configurations[13] on the step size. The precise values of the correlation length of $\langle x^2 \rangle$ change if a given run is repeated with a different random seed, but the qualitative shape of the dependence on δt is always the same. The main feature is the existence of an optimum value of the step size, where the correlation is shortest. This corresponds to an intermediate value of the acceptance: too high or too low acceptances lead to larger correlations.

We have also tested the dependence of the acceptance on the number of molecular-dynamics steps, for various values of the step size. The acceptance fluctuates around the value determined by δt (for instance, around 80% for $\mu=2$, $\delta t=0.25$ from $n=1$ up to $n=64$ molecular-dynamics steps). The corresponding correlation length is found to have a minimum around $n=1/\delta t$.

Figure 3 shows the dependence of the acceptance and of the correlation on the number of coupled oscillators (system volume). For a step size which minimizes the correlation in the corrected Langevin algorithm, we see that the acceptance drops significantly with the volume; the correlation increases sharply when the volume exceeds a certain threshold.

The fact that large step sizes and/or many degrees of freedom lead to low acceptance is not surprising for a global algorithm which suppresses large changes in the total energy. Even small local changes can accumulate to a large change in the total energy. Of course, a truly microcanonical evolution would be characterized by $\delta H=0$, but any discretization scheme of the Hamilton equations violates this condition. A large δt leads to large local changes resulting in a still larger δH. The same accumulation effect is obtained when the number of degrees of freedom increases.

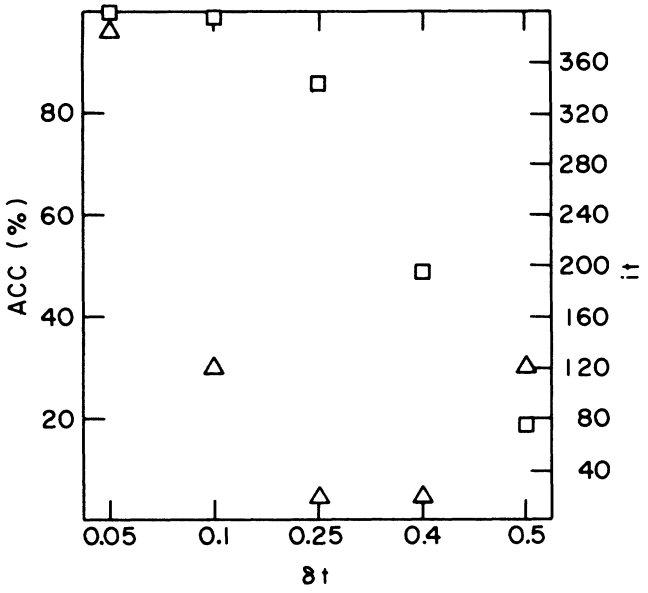

FIG. 2. Acceptance and correlation for a chain of $N=100$ coupled harmonic oscillators in function of the step size for one molecular-dynamics step. Results are obtained with the globally corrected algorithm for $\mu=2$. Squares denote the acceptance rate (left scale) and triangles represent the corresponding correlation between configurations, measured according to Ref. 13 and denoted by *it* (right scale).

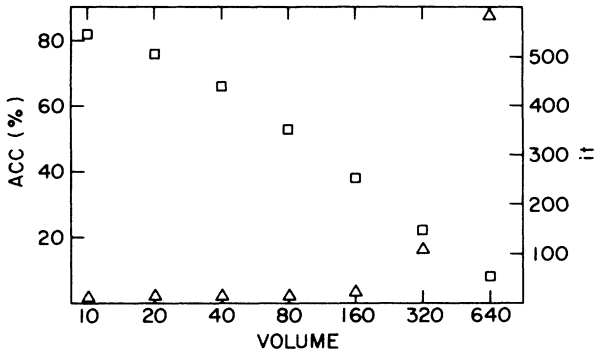

FIG. 3. Acceptance as a function of the number of coupled harmonic oscillators (lattice volume). Results are obtained with the globally corrected algorithm with $n=1$ molecular-dynamics step and $\delta t=0.4$ for $\mu=2$.

For small step sizes, the system explores phase space very slowly and almost every proposed configuration is accepted. Therefore, a large number of trajectories is needed to produce an independent configuration. On the other hand, too low an acceptance means that a very small sample of configurations is generated. These considerations qualitatively explain the observed dependence of the correlation between configurations on the step size and on the number of degrees of freedom.

IV. PURE SU(3) THEORY

Figure 4 shows the step-size dependence of the accuracy of uncorrected and globally corrected updating for pure SU(3) theory with the Wilson action (14) on a 4^4 lattice. The coupling is $\beta=4.8$ as in Ref. 5; the corridor represents the benchmark of Ref. 5. 10^4 configurations were generated for each data point. We see that the globally corrected algorithm is consistent with the benchmark for δt as large as 0.3. Thus, the violation of detailed balance due to the exponentiation error (Sec. II) appears to be insignificant for such step sizes. The uncorrected hybrid algorithm is accurate for $\delta t \leq 0.1$ but starts to deviate for larger step sizes (to compare with the results of Ref. 5, note that $\delta t=\sqrt{\epsilon}$, where ϵ is the Langevin step size).

A comparison of Fig. 5(a) and Fig. 2 reveals a similar interdependence of step size, acceptance rate and correlation between configurations. For $\delta t=0.3$, the acceptance is only 0.5% and yet the globally corrected algorithm converges to the benchmark within the set number of sweeps. This shows that very low acceptance rates are

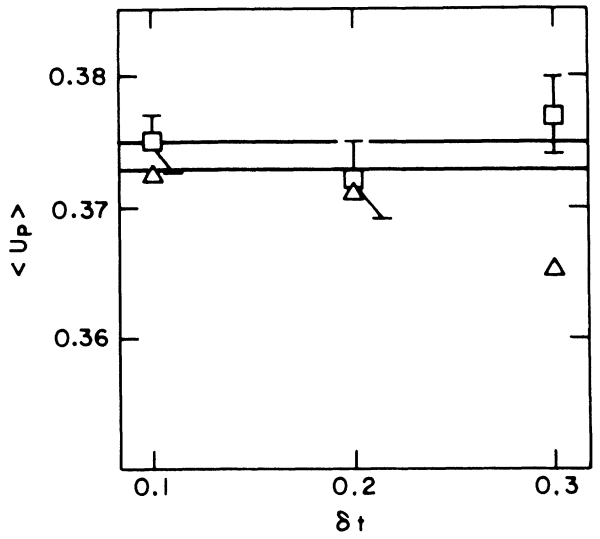

FIG. 4. Accuracy of globally corrected and of uncorrected hybrid updating for pure SU(3) theory on a 4^4 lattice. All the runs are for $\beta=4.8$. The corridor represents the benchmark obtained in Ref. 5 by means of the local Metropolis *et al.* algorithm. Squares denote the results of corrected Langevin updating ($n=1$ molecular-dynamics step) and triangles represent the results of uncorrected hybrid updating ($n=5$ molecular-dynamics steps).

not necessarily bad, provided the system is such that the corresponding correlation between configurations is not unduly large.

Figure 5(b) shows the decrease of the acceptance as the number of molecular-dynamics steps is increased. The dependence is seen to flatten out when $n>6$. The corresponding correlation[13] between Wilson loops measured on successive configurations drops by a factor 2 when we go from $n=1$ to $n=2$ and remains approximately constant (with oscillations) for larger n. When we repeat this exercise at lower step sizes, we find that all acceptances are shifted to larger values, so that the decrease of the acceptance with the number of molecular-dynamics steps is less and less pronounced. For instance, the acceptance for $\delta t=0.035$ and $n=10$ is about 80%. With a different choice of parameter values and with another variant of the leapfrog algorithm, Ref. 14 seems to obtain results which are qualitatively similar to ours.

It is obvious that the acceptance rate can be improved by minimizing the systematic error of the hybrid trial update at a given step size. It has been suggested in Ref. 9 that this could be achieved by shifting the couplings in the molecular-dynamics evolution away from the "physical" values at which the accept/reject step is taken. Indeed, the difference between the equilibrium action of the Langevin or hybrid process and the action of SU(3) can be reduced by such shifts.[2,5] One might use this observation by tuning the coupling in the tentative updating until the acceptance is maximal. This would presumably be at or near where the systematic error is minimal. However, by running the leapfrog updating algorithm with various couplings $\beta+\delta\beta$ (where the accept/reject step was taken with β), we find that the dependence of the acceptance on $\delta\beta$ shows a rather broad, unstructured maximum around a small positive $\delta\beta$. Correspondingly, the difference between the final and initial Hamiltonians showed a broad flat minimum. Thus we find no significant improvement by using $\delta\beta\neq 0$. It might be more effective to use a higher-order discretization scheme of the microcanonical equations in order to reduce the systematic errors.

To get an idea of the β dependence of the systematic errors of approximate algorithms, we have used a globally corrected Langevin run with $\delta t=0.1$ to set a benchmark above the deconfinement phase transition, at

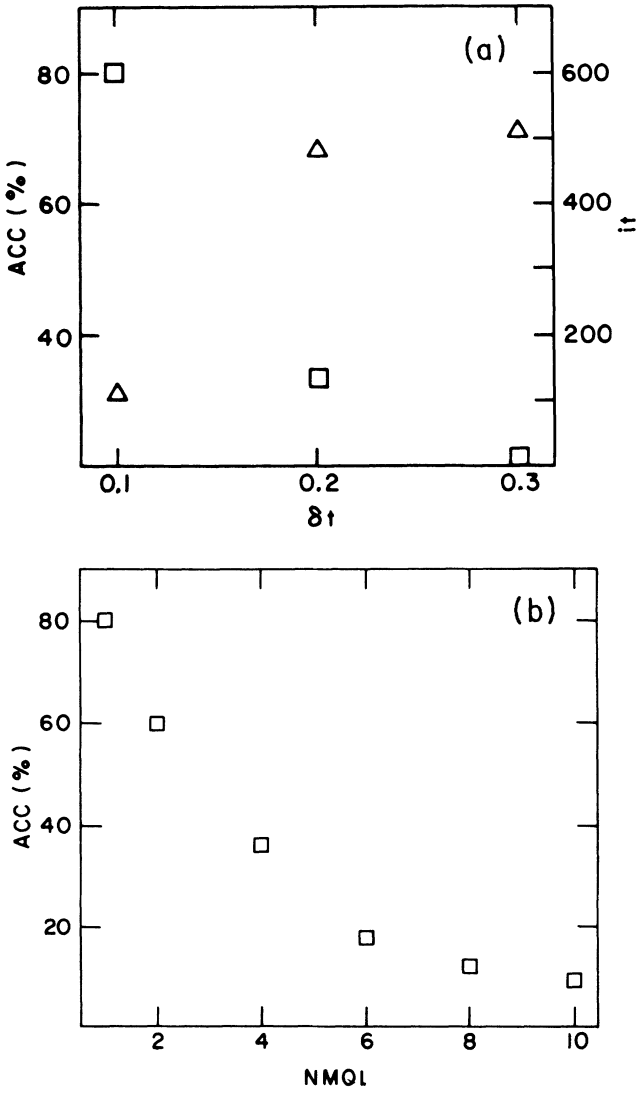

FIG. 5. Acceptance and correlation for pure SU(3) theory on a 4^4 lattice. Results are obtained with the globally corrected algorithm for $\beta=4.8$. Squares denote the acceptance rate (left scale) and triangles represent the corresponding correlation between configurations, denoted by *it* (right scale). (a) shows the dependence upon the step size for one molecular-dynamics step. (b) shows the dependence upon the number of molecular-dynamics steps for $\delta t=0.1$.

TABLE I. The globally corrected and uncorrected hybrid algorithms are compared on the basis of 1×1 Wilson loops. Quoted errors (numbers in parentheses) are corrected for correlations between configurations (Ref. 13). For SU(3), G is a globally corrected Langevin ($n=1$) with $\delta t=0.1$ and H is an uncorrected hybrid with $\delta t=0.2$ and $n=5$. For QCD the quark mass is $ma=0.1$ and $n_f=4$. G is a globally corrected hybrid with $\delta t=0.01$, $n=3$ and a residue $r=0.01$; H is an uncorrected hybrid with $\delta t=0.1$, $n=5$, $r=0.2$.

Theory	β	G	H
SU(3)	4.8	0.3752	0.3715
		(0.0018)	(0.0006)
	5.8	0.5780	0.5597
		(0.0013)	(0.0008)
QCD	4.8	0.4076	0.3956
		(0.0011)	(0.0007)
	5.2	0.5250	0.5248
		(0.0046)	(0.0011)

$\beta=5.8$. Based on our previous results, we are confident that this choice of parameters will lead to an exact result. Indeed, we find an acceptance rate of 72% and a correlation of about 170 configurations. We have then run the uncorrected hybrid algorithm with $\delta t=0.2$, $n=5$ at the same β.

As seen in Table I, the systematic error in the 1×1 Wilson loop is larger in the deconfined phase. Since the relative error only goes from about 1% to about 3%, the phase transition does not seem to induce a qualitative change in the systematic error. The deconfinement order parameter (the Polyakov loop), as measured with the uncorrected procedure, is clearly nonzero at $\beta=5.8$. (The systematic errors on this nonlocal observable are hard to quantify on a 4^4 lattice because of the large finite-size fluctuations.) Thus, the upward shift in the critical coupling which is induced by the systematic error[5] is not very large.

V. QCD WITH DYNAMICAL QUARKS

Full QCD with light dynamical quarks is of course the most challenging potential application of globally corrected updating schemes. There has been a series of investigations of the systematic errors of various approximate algorithms on a 4^4 lattice for $n_f=4$ quark flavors of mass $ma=0.1$ in lattice units at $\beta=4.8$ (Refs. 4–6 and 8). The main controversy in these studies concerns the benchmark to which the approximate results are to be compared: the results obtained with various "exact" algorithms for the 1×1 Wilson loop range from $W(1\times1)=0.416$ to $W(1\times1)=0.404$. All these results can be criticized for having small statistics and for using rather large inversion residues—these limitations being consequences of the lack of efficiency of the exact algorithms. It is interesting to see if our globally corrected hybrid algorithm can fare any better.

The combination $n=1$, $\delta t=0.1$ had produced an acceptance of 80% for pure SU(3). Upon adding the fermions, this dropped so sharply that no new configurations could be generated in a practical time span. By reducing the step size to 0.05, the acceptance was raised to about 30% but the corresponding correlation was of the order of 1000 configurations. To reduce this correlation, we increased the number of molecular-dynamics steps between momentum refreshings, but this again caused a drop in the acceptance. We finally used $\delta t=0.01$ in our runs.

The inversions of the staggered Dirac matrix M required by Eqs. (16)–(19) were all done with the conjugate-gradient method. Denoting $y=Mx$, our definition of the residue is $r=|Mx-y|$. (Note that this definition does not divide out the volume.) Even a fermionic algorithm which satisfies detailed balance will have a systematic bias if this residue is nonzero. Therefore, one would like to run with as low a residue as possible. However, as seen in Fig. 6, in our globally corrected scheme this means not only more computer time per updating step but also an additional penalty in acceptance. Figure 6 was obtained using the same residue for all conjugate-gradient inversions (in the computation of the initial and final Hamiltonians as well as in the leapfrog steps). Very similar results are obtained if one only varies the residue in the computations of the Hamiltonians while keeping the residues in the leapfrog steps fixed at 0.2.

Table I shows our result for $W(1\times1)$ after 22×10^3 globally corrected hybrid trajectories with $\delta t=0.01$, $n=3$, $r=0.01$. The average acceptance rate was $9.2\pm0.5\%$ and the correlation was about 700 configurations. The slow rate of exploration of phase space and the smallness of the lattice lead to large fluctuations at equilibrium $[W(1\times1)\in[4.00,4.20]]$. For these reasons, a longer run would be required to establish a truly reliable benchmark.

The globally corrected algorithm was run with the same parameters at $\beta=5.2$, above the QCD phase transition. An interesting feature was that the acceptance rose to about 33%, which is presumably related to the fact

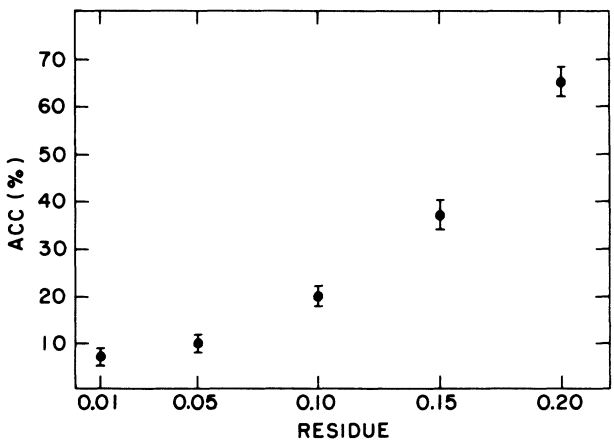

FIG. 6. Acceptance versus inversion residue for full QCD on a 4^4 lattice. Results are for $\beta=4.8$, $n_f=4$, $ma=0.1$. They are obtained with the globally corrected algorithm with $\delta t=0.01$ and $n=3$ molecular-dynamics steps.

that the number of conjugate-gradient iterations required to achieve $r \leq 0.01$ dropped from about 87 to about 60. Within the statistics of our runs, the systematic error by the uncorrected hybrid algorithm appears to be lower above the phase transition. Because of the proximity of the QCD phase transition, the correlation in this run was far larger than at $\beta=4.8$, which accounts for the larger error quoted in Table I. In any case, as for SU(3), we find that the phase transition has no dramatic effect upon the systematic error. The uncorrected algorithm reproduces the fact that the absolute value of the real part of the Polyakov loop is large at $\beta=5.2$, i.e., that the theory is in its high-temperature phase.

The fact that the acceptance decreases when the quark mass is decreased from infinity [pure SU(3)] is due to the fact that the effective step size of the noisy estimator algorithm increases when the mass is lowered.[2,5] Another factor which may contribute to the decrease in acceptance as the fermions are added is the corresponding increase in the number of degrees of freedom of the system (equivalent to an increase in volume). The decrease of the acceptance with the inversion residue may seem surprising, since one might expect that a more exact inversion would generate smaller deviations from the true equilibrium of the fermionic theory and hence a higher acceptance rate. On the other hand, inexact inversion will tend to reduce the fermionic degrees of freedom to noise, which will cancel out in the global accept/reject step. Thus, the gauge degrees of freedom will dominate the acceptance criterion, leading to a higher acceptance rate.

By comparing our results to those obtained by the background-field method,[14,15] one sees that the noisy estimator method requires lower step sizes in order to achieve similar acceptances. Thus, it seems that one must pay a price for using nondeterministic evolution equations. The large fluctuations in equilibrium and the long correlations which were our main practical problems might also be consequences of the noisy estimation of the fermionic contribution.

VI. CONCLUSIONS

We have tested globally corrected hybrid updating algorithms for various physical systems. For the coupled harmonic oscillators and for pure SU(3), we found that such algorithms work satisfactorily even at step sizes where the corresponding uncorrected hybrid algorithms have significant systematic errors. The updating step size can be chosen such as to minimize the correlation between configurations, thus ensuring an efficient exploration of phase space. However, for such bosonic theories, "classical" Monte Carlo updating remains superior.[10]

We have tried to use a globally corrected version of the noisy estimator algorithm, which is popular in uncorrected Langevin and hybrid updating, to produce long benchmark runs above and below the finite-temperature phase transition in full QCD. Advantageous acceptance rates were only obtained at rather small step sizes, which lead to large fluctuations and to long-run time correlations between observables. To a lesser extent, fermionic simulations which use globally corrected background-field updating encounter the same problem.[10,14,15] It appears that these problems become more severe as the fermion mass is decreased and as the lattice volume increases. At the small step sizes to which the corrected algorithms are thus forced, the corresponding uncorrected algorithms have small systematic errors themselves.[2,3,5]

The obvious way to improve the performance of the global algorithms is to improve the performance of the hybrid algorithm which produces the trial configurations. The idea is to reduce the departure from microcanonical evolution for a given step size by some higher-order reversible and area-preserving discretization of the equations of motion. As long as reversibility and Liouville's theorem are preserved, one is in fact free to chose any intermediate updating scheme which proves convenient. In this context, it is interesting to investigate to what extend one can save computer time by performing the inversions for the intermediate updates with less accuracy than those required for the global accept/reject step.

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