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EXPERIMENTING WITH LANGEVIN LATTICE QCD

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ABSTRACT

We report on the status of our investigations of the effects of systematic errors upon the practical merits of Langevin updating in full lattice QCD. We formulate some rules for the safe use of this updating procedure and some observations on problems which may be common to all approximate fermion algorithms.

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We report on the status of our investigations of the effects of systematic errors upon the practical merits of Langevin updating in full lattice QCD. We formulate some rules for the safe use of this updating procedure and some observations on problems which may be common to all approximate fermion algorithms.

INTRODUCTION AND SUMMARY

Understanding the origins and effects of systematic errors in the algorithms used for the numerical simulation of lattice QCD is increasingly recognized as one of the major problems in the field [1]. The updating procedure based on the discretized version of the Langevin equation [2-4] is well suited for such studies, because the origin of its systematic errors is well understood [3,4] and because the leading errors are under analytic control [2-5]. Since Langevin updating can be connected to microcanonical updating via "hybrid" algorithms [6] and to pseudo-fermion updating [7] via the procedure suggested in Ref. [8], any findings on Langevin systematic errors may also turn out to be relevant to these other procedures. This is especially likely for the specific effects of the fermion determinant.

Our numerical study of the systematic errors in Langevin algorithms for QCD with dynamical quarks [9,10] is restricted to basic (non-hybrid, real-action, non-Fourier-accelerated) updating. It takes place on a 4^4 lattice having periodic boundary conditions in 3 directions and antiperiodic ones in the fourth. The coupling is fixed to $\beta = 4.8$; we simulate four flavors of Kogut- Susskind quarks of masses $ma = 0.1$ and $ma = 0.05$ using the Cornell group's bilinear noise approach [2].

We measure planar Wilson loops at various values of the discrete step size in Langevin time. The systematic error originates in the finite value of this step size and becomes worse as the step size increases. It is interesting to assess the effect of the bias upon planar Wilson loops, because these are the fundamental building blocks of most lattice observables. Therefore, the errors on the fundamental Wilson loops will in general propagate non-trivially to plague the eventual physical quantities one wants to extract.

As a benchmark to assess the effects of the error, we use the measurements of the same loops performed with an algorithm which computes the fermion determinant directly [11]. We also compare the Langevin results to those obtained with the pseudo-fermion method at various acceptances [11]. Since the number of iterations necessary for equilibration and the size of time correlations in equilibrium are important in determining the total cost of a numerical experiment which aims for a given statistical error, we also monitor these quantities by various methods. Note that these quantities decrease as the time step increases. What we require is a procedure which allows us to run at the largest possible step size with an acceptable systematic error.

The main result we want to present here is a set of "safety rules" for Langevin updating:

1. In order to obtain Wilson loop measurements in reasonable agreement with the benchmark for quark mass $ma = 0.1$, one may choose out of three methods:

   A. One run with the first-order (Euler) algorithm using a time step $\epsilon \lesssim 0.001$. Since time correlations are rather large with this method, the run must be sufficiently long.

   B. Use the Euler algorithm, but do 2 or 3 runs in the step size interval $\epsilon \in [0.005, 0.01]$. A linear extrapolation to $\epsilon = 0$ gives a good central value for your loop.

   C. One can do one run with the second-order (Runge-Kutta) algorithm with $\lesssim 0.001$. This will give results similar to the

ones obtained by method A; time correlations will be smaller but the overall cost is slightly larger because this algorithm requires two conjugate gradient inversions instead of one.

2. For the values of the step size mentioned above, the non-integrable contribution to the leading systematic error is numerically unimportant.

3. There are physically important problems of a qualitative nature, such as the presence or absence of a first-order phase transition, which can be investigated without worrying about the systematic error. One can study these using either first order or second order algorithms, with a step size (say, $\epsilon = 0.01$) which should still be small enough that the absolute values of the monitored quantities (plaquette, $\bar{\chi}\chi$, Polyakov line) are reasonable. When using the Euler algorithm, one should shift the coupling, number of flavors and mass according to the formulae given in Refs. [2,5,10].

4. The effect of the systematic error becomes more severe when the quark mass is decreased to $ma = 0.05$. In this case, runs at $\epsilon = 0.001$ are no longer sufficient: one should go to still smaller step sizes.

2. ALGORITHMS

We shall begin by briefly reviewing the basic notations and formalism of discrete Langevin diffusion processes in SU(3) group space, the origin of systematic errors in Langevin updating and the algorithms we have been testing. Any SU(3) lattice link variable $U_\mu(x,\tau)$ (x runs over lattice sites and μ runs over Euclidean directions) is updated from Langevin time τ_N to τ_{N-1} by the formula

$$U_\mu(x,\tau_{N-1}) = U_\mu(x,\tau_N)\exp\left(-if_a T_a\right) \qquad (1)$$

where T_a are the generators of SU(3) ($a = 1,2,\ldots 8$; $trT_aT_b = \delta_{ab}/2$) and $f_a = f_a[U,\eta_x]$ is called the driving force. The driving force is built out of link matrices and out of 8 SU(3)-matrices η_x which generalize the white noise of stochastic quantization [2] ($a = 1,2,\ldots 8$; $\langle\eta_a\rangle = 0$, $\langle\eta_a\eta_b\rangle = 2\delta_{ab}$). It contains the discrete time step of the Langevin simulation, $\epsilon \equiv \tau_{N-1} - \tau_N$.

Any given choice of the driving force defines a Langevin updating algorithm for the theory. One can then use the Fokker-Planck equation associated to (1) to determine the equilibrium action $\bar{S}$ of the Langevin diffusion as a function of the QCD action S. The result is of the form [3-5]

$$\bar{S} = S + o\left(\epsilon^n\right), \qquad (n = 1,2,\ldots) \qquad (2)$$

This difference between $\bar{S}$ and S is the origin of the systematic error in Langevin updating. The explicit form of the relationship (2) can be used to engineer f_a such that the error be minimal (n in Eq. (2) maximal). Unfortunately, (2) can be worked out analytically (so far) only to first order in ϵ, so that algorithms can only be improved to yield $n = 2$ [2-5]. Therefore, numerical experiments remain the only way to assess the effects of the systematic bias upon lattice observables.

We report here on the performance of the following Langevin algorithms for full QCD:

1. First-order (Euler) QCD with fermionic noise. The driving force is [3]

$$f_a = \epsilon \left(\partial_a S_g [U] - \frac{1}{4} \xi^\dagger A_a [U] \xi \right) + \sqrt{\epsilon} \eta_a \qquad (3)$$

where S_g is the usual Wilson action,

$$A_a [U] = M^{-1} [U] \partial_a \left(M^\dagger M \right) M^{-1} [U], \qquad (4)$$

$M = D + ma$ such that $S = S_g - (1/2) Tr \ln M^\dagger M$ for 4 flavors of staggered quarks and ξ is a bilinear noise, normalized like the η_a's. This leaves $\bar{S} - S$ of order of order ϵ [3,5].

2. "Naive" second-order (Runge-Kutta) QCD with fermionic noise. This is defined by the driving force [5]

$$f_a = \frac{\epsilon}{2}(1 + \frac{C_2 \epsilon}{12})(\partial_a S_g[U] + \partial_a S_g[\tilde{U}] - \frac{1}{4} \xi^\dagger A_a[U] \xi - \frac{1}{4} \chi^\dagger A_a[\tilde{U}] \chi) + \sqrt{\epsilon} \eta_a \qquad (5)$$

where $\tilde{U} \equiv U \left(x, \tau_{N-1/2} \right)$ represents an intermediate update obtained by Eqs. (1) and (3) and χ is a second bilinear noise. The difference between $\bar{S}$ and S is now of order ϵ^2, up to a so-called "non-integrable term" which arises from averaging over the bilinear noise and which is of order $\epsilon^{3/2}$ [5].

3. A "true" second-order algorithm, which leaves only errors of order 2 and higher, can be obtained by cancelling the non-integrable term explicitly [5]. This is done by replacing η_a in Eq. (5) by

$$\bar{\eta}_a = [\delta_{ab} - \frac{\epsilon}{12} \mathrm{Re} \{ \xi^\dagger A_a \chi \chi^\dagger A_b \xi \}] \eta_b \qquad (6)$$

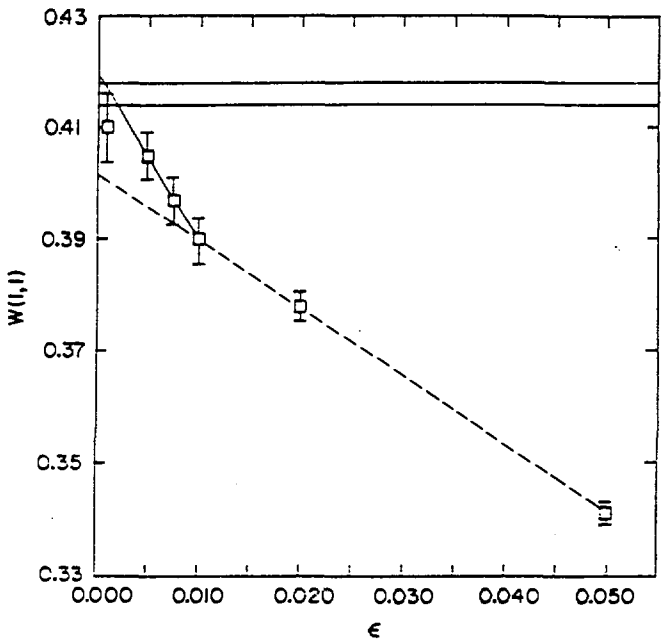

Fig. 1: Performance of the Euler algorithm for Langevin QCD. The full corridor indicates the benchmark result [11]. Error bars are corrected for time correlations in equilibrium [12]. Straight lines represent possible extrapolations.

3. THE EULER ALGORITHM

Figure 1 presents the dependence of the 1×1 Wilson loop on the step size. It has been obtained by using the Euler algorithm under the following conditions: $\beta = 6/g^2 = 4.8$, the quark mass in lattice units $ma = 0.1$, four flavors of Kogut-Susskind quarks. The inversion of M was done by conjugate gradient. We imposed the stopping condition $r = \left(||M\bar{x} - \bar{\xi}||^2\right)^{1/2} < 0.05$. Note that our definition of the residue differs from other popular definitions by not dividing out the length of the vector $\bar{\xi}$ (our $r = 0.05$ is of the order 10^{-5} in the other normalization). In the mean, the required accuracy was reached after 65 conjugate gradient iterations. The updating time per link

resulted to be about 0.88 milliseconds on the CRAY X-MP 22 at NMFECC (as compared to about 0.77 milliseconds for a similarly optimized pseudo-fermion code). Equilibration was checked in all cases by comparing averages over successive batches of 3000 iterations, for all Wilson loops up to 3×3. At $\epsilon = 0.01$ we also checked that hot and cold starts converge to the same average plaquette. The final averages were then obtained over 3000 iterations at equilibrium.

The corridor in Fig. 1 represents the result of the recent direct computation of the fermion determinant [11], which was done under exactly the same conditions as the present study. We see that we can come close to the benchmark either by running at sufficiently low ϵ ($\epsilon \lesssim 0.001$) or by doing two runs in the interval $\epsilon \in [0.005, 0.01]$ and extrapolating linearly to $\epsilon = 0$. An extrapolation based on runs below $\epsilon = 0.01$ would underestimate the value of the plaquette by far.

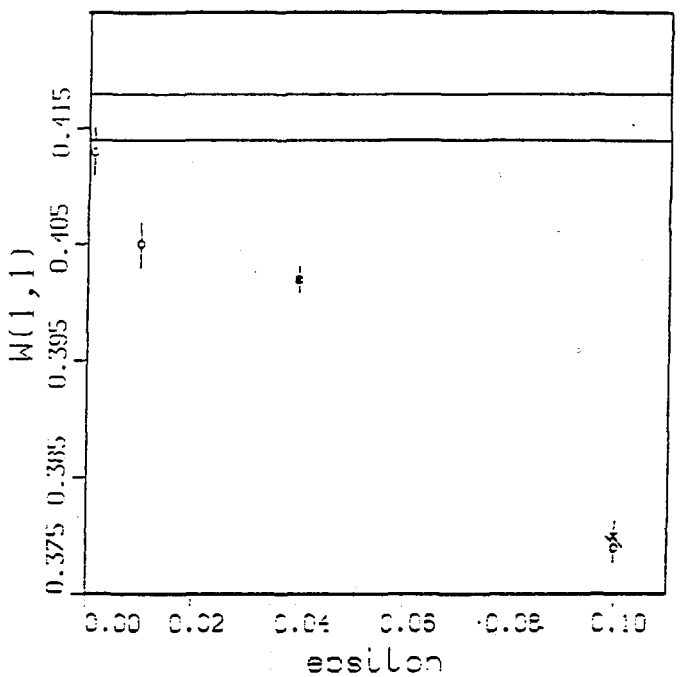

Fig. 2: Performance of Runge-Kutta algorithms for Langevin QCD. Open circles represent the results of the algorithm of Eq. (5) and crosses represent the results of Eq. (6). The full corridor shows the result of the exact computation [11].

TABLE I: Relative performance of Langevin and pseudo-fermion algorithms ($ma = 0.1$). Algorithm D is the direct computation [11], P reproduces the relevant pseudo-fermion results of [11] and L is the Runge-Kutta algorithm of (5).

Alg.		Acc.	W(1,1)	W(1,2)	W(1,3)	W(2,2)	W(2,3)	W(3,3)
D			.042 (.003)	.039 (.003)	.023 (.003)	.016 (.003)	.005 (.002)	.001 (.002)
P		.86	.042 (.002)	.039 (.002)	.024 (.001)	.017 (.001)	.005 (.001)	.001 (.001)
L	.001		.039 (.002)	.038 (.002)	.024 (.002)	.018 (.002)	.004 (.002)	.003 (.002)
P		.74	.030 (.002)	.027 (.002)	.016 (.001)	.010 (.001)	.003 (.001)	.001 (.001)
L	.01		.031 (.002)	.029 (.002)	.018 (.001)	. 011 (.001)	. 002 (.001)	.002 (.001)

4. RUNGE-KUTTA ALGORITHMS

Figure 2 contains the same information as Figure 1 for the case of the Runge-Kutta algorithms (5) and (6). Table I assesses the quality of various planar Wilson loops measured using Eq. (5) with respect to the benchmark set in Ref. [11] and with respect to the pseudo-fermion algorithm at various acceptances [11]. Using Eq. (5), one must do 2 conjugate gradient inversions per Langevin step; the updating time per link becomes about 1.65 milliseconds and the memory requirement becomes about 5/4 that for the Euler or pseudo-fermion schemes. Eq. (6) requires 3 inversions per time step and takes about 2.37 milliseconds per link update.

We see that the higher-order errors are still substantial unless $\epsilon \lesssim 0.001$, in which case both first-and higher-order errors are rather small. The improvement gained by cancelling the non-integrable term is seen to be insignificant. There appears to be a correpondence between the Langevin and the pseudo-fermion algorithms: Runge-Kutta at $\epsilon = 0.001$ is comparable to pseudo-fermions at 86% acceptance and Runge-Kutta at $\epsilon = 0.01$ to pseudo-fermions at 74% acceptance. Time correlations and hence the corrected statistical errors [12] are systematically smaller for the Runge-Kutta than for the Euler scheme. However, the total run time required to achieve a given accuracy would still be higher for the second-order scheme because of the additional matrix inversion.

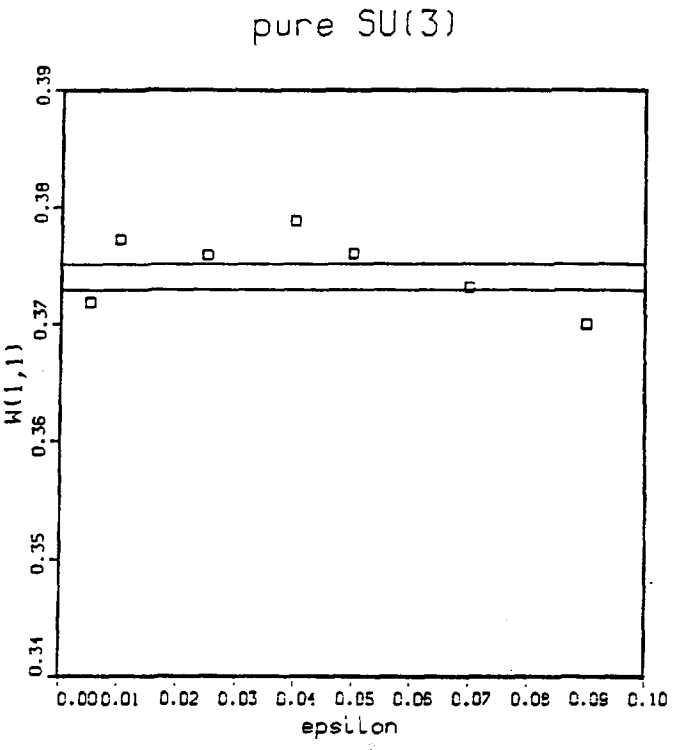

Fig. 3: The Runge-Kutta algorithm for Langevin pure SU(3). All the runs are on a 4^4 lattice with $\beta = 4.8$. The benchmark is based on runs with the standard Metropolis et al. method.

5. LOWERING THE QUARK MASS

Ref. [11] has observed that the pseudo-fermion algorithm performs less well with respect to the benchmark at quark mass $ma = 0.05$ than at $ma = 0.1$. Would this also be the case for Langevin updating? We have run the Runge-Kutta algorithm based on Eq. (5) at $ma = 0.05$ in order to answer this question. Using $\epsilon = 0.001$ and a stopping residue of 0.2 (as in [11]) which is reached after 121 conjugate gradient iterations on the average, we spend about 2.13 milliseconds per link update and find

$$\langle W(1,1)\rangle = 0.404 \pm 0.003$$

as compared to [11]

$$\langle W(1,1)\rangle = 0.417 \pm 0.002 \qquad \text{(DIRECT ALGORITHM)}$$

$$\langle W(1,1)\rangle = 0.410 \pm 0.006 \quad \text{(PSEUDO} - \text{FERMIONS 86\%)}$$

We tried lowering the stopping residue to $r = 0.01$ (reached after about 189 conjugate gradient iterations: 3.32 milliseconds per link update) but all the Wilson loops remained the same within errors (for instance, $\langle W(1,1)\rangle = 0.405 \pm 0.003$).

It would seem that Langevin at $\epsilon = 0.001$ is still comparable to pseudo- fermions at 86% acceptance and that the effective systematic error increases for both algorithms as the quark mass is decreased. That this is indeed an effect of the non-linear fermion determinant can be seen by comparing Fig. 2 to Fig. 3, which shows the ϵ-dependence of $W(1,1)$ in pure SU(3) [10]. The range of ϵ where Langevin algorithms give good results appears to shrink progressively as the quark mass decreases from infinity. This tends to confirm the observation [13] that the residual systematic error in Eq. (2), for fermionic schemes, is actually of the order ϵ^2/λ^4, where λ is some average over field configurations of the lowest eigenvalue of the lattice Dirac operator. It is known that this average decreases with the quark mass. It is tempting to speculate that the same effect is also seen in the pseudo-fermion scheme.

6. CONCLUSIONS

Our numerical experiments have shown that the analytically intractable terms of order ϵ^2 and higher in Eq. (2) have substantial effects upon planar Wilson loops in full QCD. Based on the known first-order correction terms, one had hoped that all systematic errors could either be eliminated by improving the naive Euler algorithm or they would be irrelevant in the continuum limit. Even though the quantitative insignificance of the leading-order non- integrable term is good news in this respect, the large effects of higher- order terms mean that such an optimistic conclusion cannot be taken for granted in the general case. One should therefore respect the "safety rules" we recommended above.

A study such as the present one obviously depends upon the existence of reliable and accurate benchmarks. It is therefore very important to pursue the effort initiated in [11], to make sure the direct algorithm has no significant hidden bias of its own and to improve the statistics of these benchmark runs.

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