Some aspects of simulation algorithms for dynamical fermions *

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Three topics concerning fermion simulation algorithms are discussed: 1.) A performance comparison of the multiboson technique to simulate dynamical fermions and the Kramers equation algorithm, 2.) the question of reversibility in the Hybrid Monte Carlo algorithm and 3.) the implementation of Symanzik's improvement program for dynamical Wilson fermions.

1. Introduction

Wilson's suggestion to formulate QCD on an euclidean space-time lattice opened the path to non-perturbative and first principle investigations of strong interactions. It was soon realized that for pure Yang-Mills theory numerical simulations are a powerful tool to address several questions in this theory. In particular, numerical simulations can build a bridge between the high energy regime, where perturbation theory is valid, to scales where non-perturbative effects set in.

However, as the title of this workshop already suggests, simulations with dynamical fermions have still to be accelerated in order to obtain results with small enough error bars in a reasonable amount of time. Therefore, in the last years we have seen a revived interest in a better understanding of the existing algorithms (the old work horses) as we have seen new developments.

Such a development is the multiboson technique to simulate dynamical fermions \textsuperscript{1} and we will in section 2 compare its performance to the Kramers equation algorithm \textsuperscript{2,3}. Section 3 is concerned with the question of lack of reversibility in the Hybrid Monte Carlo algorithm \textsuperscript{4} which may cause potential problems with the detailed balance condition in practical simulations. The 4th section will contain a short account of the implementation of Symanzik's improvement program for Wilson fermions. The overhead due to the addition of the extra Sheikholeslami-Wohlert (SW) term \textsuperscript{5} in the lattice action will be discussed. Note that in sections 2 and 3 the gauge group is chosen to be SU(2) while in section 4 it is SU(3).

Space limitations do not allow to give here a full account of all the notations and background. For this we have to refer to the original literature \textsuperscript{3,4,6,7}.

2. Performance comparison of the multiboson technique to simulate dynamical fermions and the Kramers equation algorithm

In this section, the performance of two algorithms is compared. The first one goes back to a suggestion of Horowitz \textsuperscript{2} and is called the Kramers equation algorithm \textsuperscript{2,3}. In a free field analysis it gives the same value of the dynamical critical exponent, $z = 1$, as the Hybrid Monte Carlo (HMC) algorithm \textsuperscript{4}. However, whereas in the HMC algorithm this value of $z$ is only reached in the limit of a large number of molecular dynamics steps, the Kramers equation algorithm needs only one step. The second algorithm is based on a new technique that makes use of the fact that

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the QCD partition function can be rewritten as a path integral of—in principle—infinitely many boson fields with interactions given by the fermion matrix on the lattice. Fortunately enough, it turned out that for practical simulations only a moderate number of these boson fields is required to obtain a good approximation of the QCD partition function \cite{9}. The tests of the Kramers equation algorithm and the multiboson technique have been performed for Wilson fermions. For a detailed description and investigation of the two algorithms see \cite{6} and \cite{3}. For alternative realizations of the multiboson technique see \cite{11} and for a review \cite{10}. Let us here only emphasize the improvements over the “bare” algorithm that we have installed. Starting with the Kramers equation algorithm, we

- installed standard even-odd preconditioning \cite{12}
- and used a particular integration scheme that allows for larger step sizes \cite{13}.

For the multiboson technique we

- used again even-odd preconditioning,
- introduced a normalization factor for the fermion matrix that lifts the lowest eigenvalue while keeping the largest one below one \cite{11,6}
- and made a careful investigation of the optimal choice of the mixing ratio of heatbath and over-relaxation updates \cite{6}.

Let us mention that each of the above improvements may lead to substantial factors of accelerating the program. We also looked at the chronological extrapolation method to find better starting vectors for the conjugate gradient algorithm \cite{14}. However, due to the use of large step sizes in the Sexton-Weingarten integration scheme, we did not find a further acceleration of the program in our case.

The algorithm and coupling parameters used for the tests may be found in \cite{4}. We worked at a rather large pion to $\rho$-mass ratio of 0.95. All numerical simulations have been performed on the Alenia Quadrics (APE) massively parallel machines. In table 1, we give the time $\tau$ in real seconds that the algorithms need to generate an independent configuration. The subscript $b$ stands for the multiboson technique and $k$ for the Kramers equation algorithm. The computationally most expensive part in the Kramers equation algorithm is the conjugate gradient method for the matrix inversion. This inversion, on the other hand, is dominated by fermion matrix $Q$ times vector $\phi$ operations, denoted by $Q\Phi$. Also for the bosonic algorithm similar floating point operations dominate the program \cite{11,6}. For this reason we give the autocorrelation time $\tau(Q\Phi)$ in units of $Q\Phi$ in columns 3 and 4 which is a more machine independent measure of the performance.

We see that within the error bars for the autocorrelation time, both algorithms show a comparable performance.

3. Reversibility

In order for the HMC algorithm to fulfill the detailed balance condition, reversibility of the equations of motion has to hold. However, problems with the reversibility condition have been encountered and in this section some aspects of these problems will be discussed.

In the HMC algorithm the fields are evolved according to a non-linear first order stochastic differential equation. In the continuum, such differential equations are candidates for describing the time evolution of a classical chaotic system. Of course, for the computer, the differential equation has to be discretized. Nevertheless, one might expect that for small enough discrete step sizes one is close enough to the continuum and that one would observe a chaotic behaviour. To test this proposal, let us define a quantity, $||dU||$, to measure the difference between two gauge field configurations

$$||dU||^2 = \frac{1}{4\Omega}\sum_{x,\mu,a} (U^a_\mu(x) - V^a_\mu(x))^2 .$$

(1)

Here $U^a_\mu(x), V^a_\mu(x)$ are two SU(2) gauge link variables with lattice point index $x$, direction $\mu$ and group index $a$. $\Omega$ is the lattice volume.
ing errors appearing in the course of the simulation may be violated in practical simulations. Round-off errors around 0.03 were extracted. To show that this suggested chaotic behavior is really a property of Hamilton’s equations of motion, we proceeded in the following way. Given a gauge field configuration obtained in the course of some run, we added a small noise \( \delta U'_\mu(x) \) to the gauge field variable \( U'_\mu(x) \), such that \( V'_\mu(x) = U'_\mu(x) + \delta U'_\mu(x) \). Then, we took both configurations and iterated them according to the leapfrog integration scheme used in the HMC algorithm. We measured \( \|dU\| \) after some number of steps \( N_{md} \) in the leapfrog integration. If the system is chaotic, we expect that asymptotically (\( \epsilon N_{md} \gg 1 \))

\[
\|dU\| = A e^{\nu \epsilon N_{md}}. \tag{2}
\]

In eq. (2) \( \nu \) is the –to be determined– Liapunov exponent, characterizing a chaotic system and \( \epsilon \) is the step size used in the program.

Indeed, in [3] the asymptotic exponential growth of \( \|dU\| \) was verified and a positive Liapunov exponent \( \nu \approx 0.75 \) was extracted. To see whether this effect also happens in a real Monte Carlo run with dynamical Wilson fermions using the HMC algorithm we did the following: When a trajectory has been integrated, we reversed the time and integrated back, measuring \( \|dU\| \) using the initial configuration before starting the leapfrog integration and the final configuration at the end of the reversed trajectory. By fixing the step size \( \epsilon = 0.03 \), we obtained \( \|dU\| \) as a function of the trajectory length \( \epsilon N_{md} \). Indeed, we find again a linear behavior of \( \lg(\|dU\|) \) with a Liapunov exponent around 0.75. A similar observation has been made in the case of SU(3) gauge fields [5].

An important consequence of this observation is that the necessary condition of reversibility in the detailed balance proof of the HMC algorithm may be violated in practical simulations. Rounding errors appearing in the course of the simulation are blown up exponentially and destroy the reversibility of Hamilton’s equations of motion. We tried to estimate, how serious this effect is for a real simulation. We ran two HMC programs simultaneously: One with 32 bit arithmetic but with all scalar products, dot products etc. in double precision (which mirrors the case of the APE version of our program). The second one running with complete 64 bit arithmetic. The Metropolis decision in the HMC algorithm is on \( \Delta H \), i.e. the difference of the start and the end Hamiltonian. We measured the difference \( \delta(\Delta H) \) between \( \Delta H \) of the program with 32 bit and 64 bit precision. This was done for each step in the evolution \( \delta(\Delta H)_{\text{step}} \) and for a complete trajectory, \( \delta(\Delta H)_{\text{traj}} \). We find that on a \( 16^4 \) lattice \( \delta(\Delta H)_{\text{traj}} \) to be larger than \( \delta(\Delta H)_{\text{step}} \), indicating that indeed a growth of the errors due to the chaotic nature is showing up.

Repeating this test on lattices of sizes \( 8^4 \), \( 12^4 \) and \( 16^4 \), we found that by a simple extrapolation in the lattice size, for a \( 32^4 \) lattice the ratio \( \delta(\Delta H)_{\text{traj}}/\Delta H \approx 0.05 \), whereas \( \delta(\Delta H)_{\text{step}}/\Delta H \approx 0.01 \). We believe that a difference of \( \Delta H \) between the 32 bit and the 64 bit program versions reaching this level, may lead to observable effects in physical quantities.

### 4. Implementation of Symanzik’s improvement program

Following Symanzik [16], in order to cancel the \( O(a) \) effects in physical on-shell observables, it is sufficient for Wilson fermions to add a term suggested by Sheikholeslami and Wohert [6], henceforth called a SW-term. In [17], it has been demonstrated in the quenched approximation that the \( O(a) \) effects are substantial for Wilson fermions. There it was also shown that

| Lattice | machine size | \( \tau_b(Q\Phi) \) | \( \tau_b(Q\Phi) \) | \( \tau_b(\text{sec}) \) | \( \tau_b(\text{sec}) \) |
|---------|--------------|----------------|----------------|----------------|----------------|
| \( 6^4 \) | Q1 [8 nodes] | 14000(800) | 21000(4000) | 298(20) | 480(100) |
| \( 8^4 \) | Q1 [8 nodes] | 36000(2250) | 17000(5000) | 1781(112) | 979(300) |
| \( 16^4 \) | QH2 [256 nodes] | 56000(18600) | 26000(11000) | 990(330) | 480(100) |

Performance comparison of the Kramers equation and the boson algorithms. Subscripts \( b \) and \( k \) stand for the multiboson technique and the Kramers equation algorithm, respectively.
for a complete cancellation of $O(a)$ effects a non-perturbative determination of the coefficients multiplying the improvement terms is necessary. Given the experience of this work, it is a very natural next step to also implement the SW-term for dynamical fermions. The force according to the SW-term can be derived straightforwardly and it can be shown that even-odd preconditioning can be maintained. For a detailed description of our implementation and the design of possible tests of the code see [7].

When comparing with the conventional Wilson QCD simulation, the timing of the version with the improved fermion action is the crucial piece of information.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{The CPU time for the algorithm of the improved action is plotted as a function of the number of conjugate gradient iterations per step ($N_{CG}$) relative to the conventional Wilson fermion simulation. The solid and the dashed lines correspond to the choice of $t^{(0)}_w = 0$ and $t^{(0)}_w = 50$ in eq. (3) respectively.}
\end{figure}

In a typical QCD simulation using molecular dynamics algorithms, the conjugate gradient (CG) iterations dominate the CPU time of the program. Therefore, in the limit of number of conjugate gradient iterations $N_{CG}$ going to infinity, the time of the matrix-vector multiplication is the most crucial part. In our version of Symanzik improvement, this multiplication turns out to be only slightly slower than the conventional Wilson case by about 15 percent. The force evaluation, in this case, adds some overhead to the program which does not depend on $N_{CG}$. It is convenient to express all times in units of the matrix-vector multiplication of the conventional Wilson case.

To be specific, we propose the following formula for the time of the program:

\begin{align}
T_{Wilson} &= t^{(0)}_w + (t^{(1)}_w + t^{(2)}_w) N_{CG}, \\
T_{SW} &= t^{(0)}_{sw} + (t^{(1)}_{sw} + t^{(2)}_{sw}) N_{CG}.
\end{align}

In the above formula, the coefficient $t^{(2)}_w = 2$ is, by definition, the number of matrix-vector multiplications needed for each CG iteration in the conventional Wilson case. The coefficient $t^{(1)}_w$ represents the cost of other operations for each CG iteration (linear combinations, inner products etc.). Typically, this coefficient is quite small. The coefficient $t^{(0)}_w$ is the overhead that does not depend on $N_{CG}$. The value of $t^{(0)}_w$ depends on the implementation of the program. However, in the asymptotic region where $N_{CG}$ is large, the effect of $t^{(0)}_w$ becomes irrelevant.

The quantities $t^{(0)}_{sw}$, $t^{(1)}_{sw}$ and $t^{(2)}_{sw}$ are the corresponding coefficients for the program with the Sheikholeslami-Wohlert action. In this case, $t^{(2)}_{sw} = 2.3$ is slightly larger than the corresponding value in the Wilson case. The value of $t^{(1)}_{sw} = t^{(1)}_w$ remains the same and we find, for our implementation of the SW-term on the APE computer, the coefficient $t^{(0)}_{sw} \sim (50 + t^{(0)}_w)$ to be larger than that of the Wilson case. In Fig. [1] we plot the CPU time of our program with improved fermions relative to the conventional Wilson case as a function of the number of CG-iterations per molecular dynamics step. The solid and dashed curves in the figure correspond to the choice of $t^{(0)}_w = 0$ and $t^{(0)}_w = 50$ respectively, which we consider to be two rather extreme cases. For typical simulations, the curve should lie between these two. In any case, we see that, for the most interesting physical situation in which $N_{CG} \sim 200$ or more, the simulation with improved fermions is only about 20\% slower, quite independent of the value of $t^{(0)}_w$. 

5. Conclusions

We presented a performance test of the multiboson technique to simulate dynamical fermions and the Kramers equation algorithm. We find that these two quite different simulation techniques for fermions give a comparable performance. Approaches to make the multiboson technique exact by adding a Metropolis step are promising: The number of boson fields can be chosen to be small while keeping large acceptance rates [11]. A detailed performance comparison of a version of an exact multiboson program and the Kramers equation or HMC algorithm is, however, not yet available.

Possible problems with the lack of reversibility in the discretized Hamilton’s equations of motion have been discussed in section 3. A rough estimate leads to the conclusion that on lattices with size $32^4$ on machines with 32 bit arithmetic the lack of reversibility can give serious problems. For the Kramers equation algorithm this problem is substantially reduced, since one only would need one molecular dynamics step.

Coming back to the title of the workshop, did we now accelerate the fermion algorithms? The answer is yes and comes from a quite unexpected direction. The SW-term as required by Symanzik’s improvement program can be implemented straightforwardly for Wilson fermions. Fig. 1 demonstrates that the slow down of the program is only about 20%. On the other hand, by determining the coefficients multiplying the improvement terms non-perturbatively, all $O(a)$ effects in physical on-shell observables can be eliminated which results in a much faster approach to the continuum limit, in which we are most interested in.

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