Recent Developments in Fermion Simulation Algorithms

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A summary of recent developments in the field of simulation algorithms for dynamical fermions is given.

1. Introduction

Since Kennedy's complaint that there has been little activity and progress in the field of fermion simulation algorithms, we have seen much work devoted to this algorithmic challenge lattice field theory has to face. The most prominent one is Lüscher's suggestion to use a reformulation of the QCD partition function in terms of a number of bosonic field copies. This multiboson technique to simulate dynamical fermions has been studied thoroughly in the last years and it was established to lead to an exact algorithm which is competitive to the so far most often used Hybrid Monte Carlo (HMC) algorithm or its variant, the Kramers equation or L2MC algorithm.

On the other hand, with the introduction of the multiboson technique, a renewed interest to accelerate also the HMC algorithm was stimulated. Better preconditioner, as discussed by Frommer at this conference, improved integration schemes and alternative choices of matrix inverters led to a considerable amount of progress. On the negative side possible problems with the reversibility condition of the HMC algorithm has been encountered. Finally, simulations of dynamical fermions with Symanzik improved actions have already been started.

In this review talk fermion simulation algorithms for lattice QCD in the Wilson formulation are studied. For lack of space, I have to refer to e.g. for the necessary notations and definitions.

2. The algorithm race

The question one is presumably most interested in, is, which of the partly conceptually very different but exact algorithms is the fastest in the sense that an independent configuration is generated within a given amount of computer time. To find an answer, we will compare particular implementations of the multiboson technique against the HMC or the Kramers equation algorithm.

The last mentioned algorithm is a variant of the HMC algorithm. In the continuum the fictitious time evolution is described by a set of formal stochastic differential equations in the fields \( \phi \) and their conjugate momenta \( \pi \),

\[
\dot{\pi} = -\frac{\partial H}{\partial \phi} - \gamma \pi + \eta(t); \phi = \pi. \tag{1}
\]

In eq. (1) \( H \) denotes the Hamiltonian and a friction term with a coefficient \( \gamma \) appears that can be tuned to optimize the algorithm. A Gaussian noise \( \eta \) is fed into the time evolution of the system at each time step. A recent free field analysis of generalized molecular dynamics algorithms like the Kramers equation has been done in [23]. In the case of Wilson fermions the performance of the Kramers equation is comparable to the HMC algorithm [16]. For staggered fermions the situation seems to be more favorable for the HMC algorithm [24], although no definite conclusion can be given at the moment.

2.1. Scaling of the algorithms

In order to compare the performance of the algorithms, one would like to understand their scaling behaviour better. In this review, I will choose the lowest eigenvalue \( \lambda_{\text{min}} \) of \( Q^2 \) ( \( \sim M^T M \) with \( M \) the Wilson-Dirac operator) and the volume
of the lattice as the relevant scaling variables. Note that for staggered fermions the corresponding \( \lambda_{\text{min}} \) would be directly proportional to the quark mass squared. The choice of \( \lambda_{\text{min}} \) seems to be natural if one has the Schrödinger functional (SF) formulation \[25\] in mind, where simulations at zero quark masses are possible while \( \lambda_{\text{min}} \) remains non-zero \[26, 27\].

number of fields/CG iterations
The accuracy \( \delta \) of the (Chebyshev) polynomial \( P \) approximation in the multiboson technique is exponential, \( \delta \sim \exp\{-2\sqrt{n}\} \[2\]. Since \( \epsilon \) has to be chosen according to the value of \( \lambda_{\text{min}} \), in order to have a fixed accuracy the number of boson fields \( n \sim 1/\sqrt{\epsilon} \sim 1/\sqrt{\lambda_{\text{min}}} \).

The number of fields as a function of \( \lambda_{\text{min}} \) can be compared to the number of iterations needed in the molecular dynamics algorithms to invert the matrix \( Q^2 \). Fig. 1 shows the time per call of the matrix inversion routine in –for this discussion– irrelevant units as a function of the condition number \( k = \lambda_{\text{max}}/\lambda_{\text{min}} \), with \( \lambda_{\text{max}} \) the largest eigenvalue of \( Q^2 \).

![Figure 1. Time spent in the matrix inversion routine for the CG (full circles) and the BiCGstab (open circles).](image)

For the inversion the CG and the BiCGstab \[28\] methods have been used. The double logarithmic plot shows that both methods are compatible with a linear behaviour and that they basically require the same amount of computer time for the matrix inversion. Note that the condition number is ranging over several orders of magnitude. The slope of the straight line in fig. 1 is roughly 0.43 and therefore somewhat better than the expected behaviour \[29\].

An important remark is that for a smaller value of \( \beta = 5.4 \) we find, in accordance with \[28\], that the BiCGstab shows a gain of about 15-20% in spite of the fact that Schrödinger functional boundary conditions have been used. The observation that at \( \beta = 5.6 \) a comparable performance is seen, indicates that the competetivity of the two methods depends on the parameters chosen.

autocorrelation times
Little to nothing is known about the scaling of the autocorrelation time with respect to \( \lambda_{\text{min}} \). I take therefore the freedom of having an optimistic point of view and adopt the free field results for all the algorithms. This amounts to have an autocorrelation time \( \tau \sim 1/\sqrt{\lambda_{\text{min}}} \). For the multiboson technique one expects this behaviour for an optimized Hybrid-over-relaxation algorithm. For the HMC algorithm the same behaviour is found in the limit of long trajectories \[30\]. The Kramers equation algorithm assumes this with an optimal choice of \( \gamma \) for a single step trajectory \[13\].

additional scaling factors
Both type of algorithms show, unfortunately, an additional dependence on the lowest eigenvalue. For the multiboson technique it is by now well established that the autocorrelation time has a linear dependence on the number of boson fields and therefore \( \tau \sim n \sim 1/\sqrt{\lambda_{\text{min}}} \) \[4–6, 9\].

In the molecular dynamics kind of algorithms it is the tuning of the step size \( \delta \tau \) to keep a constant acceptance that gives rise to an additional scaling factor. One finds, assuming an integrator with \( \delta \tau^3 \) error \[31\] that \( \delta \tau \sim 1/\lambda_{\text{min}}^{3/4} \) for the HMC algorithm and by similar arguments \( \delta \tau \sim 1/\sqrt{\lambda_{\text{min}}} \) for the Kramers equation algorithm. Using improved integration schemes will, of course, soften this behaviour.

volume dependence
For the multiboson technique one expects a volume \( V \) behaviour as \( V (\log V)^2 \) \[4–6\]. The \((\log V)^2\) appears in the exact version of the algorithm that
is discussed below. To have a constant acceptance in this algorithm, the accuracy $\delta \sim 1/\sqrt{V}$. Therefore the number of fields $n \sim \log V$ and since the autocorrelation time scales with $n$ we finally find the $(\log V)^2$ behaviour.

The volume dependence in the molecular dynamics kind of algorithms comes basically from the acceptance behaviour. The free field analysis \([30]\) gives $P_{\text{acc}} \sim \text{erfc}(N_{\text{md}}\delta r^3\sqrt{V})$, where $N_{\text{md}}$ is the number of molecular dynamics steps. From this it follows that the HMC algorithm with $\delta r N_{\text{md}} = 1$ gives a $VV^{1/4}$ behaviour whereas the Kramers equation algorithm with $N_{\text{md}} = 1$ should give $VV^{1/6}$. For a fixed acceptance rate one finds in practise that the scaling of the step size does not contradict the theoretical estimate.

2.2. Tune up of the algorithms

There are several improvements that can be done to accelerate the “bare” algorithms. The most important of these is preconditioning the fermion matrix.

preconditioning
Using the standard even/odd preconditioning \([32]\) one not only finds that the lowest eigenvalue is increased by a factor of roughly four but that at the same time the largest eigenvalue is lowered by a factor of about two. This leads to a factor of about 8 improvement for the condition number.

The consequence for the multiboson technique is that the number of fields is decreased whereas in the molecular dynamics algorithms the number of iterations for the matrix inversion is substantially reduced.

update
For the update parts of both simulation methods it turns out that for the multiboson technique one has to optimize the mixing ratio of heatbath and over-relaxation sweeps \([34]\). In the case of the molecular dynamics algorithm a better integration scheme as suggested by Sexton and Wein- garten \([33]\) gives considerable improvement \([16]\).

matrix inversion
At the time of the conference a comparison between an exact version of the multiboson technique in its hermitian and non-hermitian variant is missing. Therefore no definite conclusion about which polynomial to choose can be given.

On the side of the molecular dynamics algorithms, it seems that the CG and the BiCGstab methods show a comparable performance for the inversion of $Q^2$ whereas the minimal residual is doing somewhat worse. Using a higher order integration scheme allows to choose larger step sizes. It seems therefore to me that for present applications there is no real need to use the chronological extrapolation method \([35]\). If, on the other hand, one reaches situations where the step size becomes small, this way of finding a good starting vector might become relevant.

It seems that for the inversion of $Q^2$ the CG algorithm is optimal. Therefore the only improvement on this side may come from better preconditioning techniques like the Oyanaga ILU preconditioning in combination with the Eisenstat trick \([35]\). An interesting idea is to use this to precondition the fermionic force \([35]\) which would allow for larger step sizes. It was suggested that one might increase the stopping criterion of the inversion routine by several orders of magnitude \([35]\) from $||r|| = 10^{-8}$, a standard choice, to $||r|| = 10^{-3}$ which still provides a reasonable acceptance rate.

Of course, by doing this, one has to choose the starting vector for the inversion to be always the same in order to guarantee the reversibility of the algorithm. It is, however, unclear to me, whether the drastic change of the residuum by five orders of magnitude will not lead to reversibility problems in practical simulations.

2.3. Making the multiboson technique exact

There have been several proposals to make the multiboson technique exact \([3,4]\). However, I consider the suggestion in \([3]\) the most promising one. One can write the exact partition function with the local bosonic action $S_b$ in the form

$$Z = \int DU \int D\Phi D\Phi |\text{det}(MP(M))|^2 e^{-S_b-S_b}. \tag{2}$$

The correction factor $|\text{det}(MP(M))|^2$ can be written in terms of new Gaussian fields $\eta$,

$$\int D\eta^\dagger D\eta e^{-[|MP(M)|]^{-1}\eta^2} \equiv \int D\eta^\dagger D\eta e^{-S_\eta}. \tag{3}$$
which defines the correction action $S_C$. The next step is to impose an accept/reject step on the correction action $S_C$. In order not to calculate the determinant factor which appears because we are considering probability densities, one has to “order” the gauge fields. We say that $U$ succeeds $U'$, $U \succ U'$, if $S_g(U) \geq S_g(U')$.

The probability $P = P_{\eta \rightarrow \eta'}(U, U')$ is then

$$P = \begin{cases} \frac{1}{|\text{det}(M_T(M))|} e^{-S_C(U, \eta')} & \text{if } U \succ U' \\ \frac{1}{|\text{det}(M_T(M))|} e^{-S_C(U', \eta')} & \text{if } U \prec U' \end{cases}$$

This probability density guarantees that in the accept/reject step the determinants cancel. In [9] the detailed balance proof of the above scheme is given. A nice feature of this approach is that one can estimate the acceptance rate analytically and the data seem to obey this analytical form in a convincing manner [9].

2.4. Performance comparison

The two kinds of algorithms have been compared for two situations. The first one is for QCD with gauge group SU(2) [10]. Here a hermitian polynomial was chosen and no Metropolis test was employed. However, the algorithm parameters were chosen such that the observables agree.

On the molecular dynamics side, the Kramers equation algorithm was used. The tests are performed at a rather large pion to $\rho$-mass ratio of $m_\pi/m_\rho = 0.95$. On the other hand, several lattice sizes $6^3 12, 8^3 12$ and $16^4$ were taken. The second test has been performed by A. Galli, C. Liu and myself with SU(3) as the gauge group. Here the multiboson technique had the exactness step implemented and its non-hermitian version was chosen. The comparison was done on a $8^4$ lattice at $\beta = 5.6$ and $\kappa = 0.1585$ which corresponds to the critical value [36]. It is gratifying to see in this case that without any extrapolation the numbers of the multiboson simulation come out to be completely consistent with the HMC value.

In fig. 2 the integrated autocorrelation times for the plaquette in more machine independent units of matrix times vector, $Q\Phi$, operations is shown for the two test cases. Given the large error bars, one can say that the algorithms perform comparably. It is surprising that the decrease of $\lambda_{\text{min}}$, when going from SU(2) to SU(3), does not seem to increase the autocorrelation time.

3. More participants in the race

In this section I will shortly describe alternatives to the algorithms described above.

bermions

Bermion simulations [37] are done at negative flavour numbers $n_f$. This at first sight strange idea appears to be very fruitful in practise. The major step forward in this approach is to impose non-perturbative matching criteria to relate the different negative quark flavours to zero and finally to, say, $n_f = 2$. During the course of investigating the bernion method, the authors also found a nice way to compute propagators in terms of pseudofermions.

The bernion approach can certainly serve to explore the parameter space as they are much cheaper than a full QCD simulation. As such they can give a very good first guess and guide the choice of parameters. Of course, at the end one would like to perform a real simulation with positive $n_f$ in order to verify the result. An open question in the bernion approach is, whether there exists a value of the quark mass at which the bernion method breaks down.

domainwall fermions
It was first pointed out in [38] that the idea of domainwall fermions, originally invented to shed light on the problem of chiral fermions on the lattice, could also be used for simulations of lattice QCD. At least for an infinite extent of the extra dimension, required in the domain-wall fermion approach, the quark mass gets only a multiplicative renormalization. Tests in the vector Schwinger model [39,40] seem to indicate that in practise one might end up with only a moderate number of slices of the extra dimension to approach the chiral limit. It is, however, too early to say, whether domainwall fermions can lead to a competitive method for full QCD simulations.

**Supersymmetry**

It is interesting to see that supersymmetry with Majorana fermions in the adjoint representation is now attacked on the lattice. The pioneering work by Montvay [41] used the multiboson technique to setup a simulation program. There, a particular construction of the polynomial in a two step procedure to approximate the Pfaffian was given. From the point of view of this review talk it is intriguing that the results by Montvay have been recalculated [42] by using a Hybrid molecular dynamics algorithm and a comparable performance of both algorithms have been found. Of course, the Hybrid molecular dynamics approach has errors \((\delta \tau)^2\) and one would therefore prefer an exact version of the multiboson technique.

There are additional attempts like Slavnov’s way of bosonization of the fermion action [43] or the approach by Liu and Thron to get rid of the pseudofermions altogether [44]. But these works are at a very early stage and one has to wait in order to see their benefits. The attempts to use adaptive step size methods seem not to lead to further progress [45]. A final but important remark is that with the multiboson technique simulations with \(n_f = 1\) might be feasible [46].

4. **Reversibility**

In order for the HMC algorithm to be exact, the equations of motion used therein have to be reversible. Although this is certainly the case for a computer with infinite precision arithmetic, in daily life one has to face rounding error effects. Indeed, it was noticed that in practical simulations the reversibility condition is not satisfied [18]. Moreover, in [16] it was pointed out that the equations of motion as used in the HMC algorithm are chaotic in nature and have a positive Liapunov exponent \(\nu\).

This implies that rounding errors eventually become exponentially amplified. The values of the Liapunov exponents have been studied as a function of the parameters \(\beta\) and \(\kappa\) [22,23]. Whereas the \(\beta\) dependence is noticeable, the \(\kappa\) dependence appears to be rather weak. In [21] it was suggested that the Liapunov exponent scales like the correlation length \(\xi\) such that \(\nu \xi = \text{const}\). One has to see, whether this interesting hypothesis will withstand future tests.

At the moment no quantitative estimate of the exponential amplification of rounding errors can be given as far as physical observables are concerned. However, estimates [22,52] indicate that one might face problems on lattice sizes larger than \(32^4\) with 32 bit arithmetic. There the reversibility error might reach a level of several percent.

5. **Symanzik improvement**

During the conference, the use of improved actions has certainly been a major topic. The investigations of the effects of improvement have so far been restricted to the quenched approximation. It is a natural and necessary next step, to implement improved actions also for dynamical fermions.

Here I want to concentrate only on the Symanzik on-shell improvement program [47]. Following this program leads to the introduction of a Sheikholeslami-Wohlert (SW) term as suggested in [48]:

\[
S_{sw} = \frac{i}{4} c_{sw} \sum_{x, \mu, \nu} \bar{\psi}(x) \sigma_{\mu\nu} F_{\mu\nu}(x) \psi(x). \tag{5}
\]

For the implementation of the SW-term in the molecular dynamics algorithms, HMC and Kramers equation, one needs to find the equations of motion while preserving even/odd preconditioning. These equations can straightforwardly be derived [49,51]. A complete implementation
of the SW-term in a dynamical fermion simulation program has been done in [50]. There are also possible tests of the code, using strong coupling expansions for the plaquette and $F^2$ are given. An independent complete implementation for the case of finite temperature simulations has been done at SCRI [51].

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Figure 3. Ratio of the time needed for the SW-action as compared to standard Wilson fermions.

Of course, the crucial question is, whether the overhead of the SW-term as compared to standard Wilson fermions appears to be small enough to justify its use in practical simulations. In fig. 3 the time overhead of the SW-action is plotted. The true time for a particular implementation should lie between the two limiting curves [50]. In any case, one notices that for a situation where the number of iterations in the inversion routine $N_{CG}$ exceeds roughly 250, the overhead is only about 20%. One should remark that it is still an open question, how the SW-term can be implemented in a simulation program using the multiboson technique if one wants to keep heatbath or over-relaxation methods for the updates.

6. Conclusion

Contrary to the situation 3 years ago, we now have two exact methods to simulate dynamical fermions at our disposal which perform competitively. The theoretical cost of the multiboson technique expressed in terms of $\lambda_{min}$ and $V$ is $V(logV)^2/\lambda_{min}^{3/2}$. This can be compared to the cost of the molecular dynamics algorithms where one finds $VV^{1/4}/\lambda_{min}^{7/4}$ for the HMC and $VV^{1/6}/\lambda_{min}^{3/2}$ for the Kramers equation algorithm. Of course, one should keep in mind that the multiboson technique has a large memory requirement and might therefore not be suitable for particular machines.

The real world situation of comparing the two kind of algorithms is summarized in fig. 2. It demonstrates that for the points investigated so far no clear priority for one or the other algorithm can be given. It would certainly be important to have more data points. I also consider it urgent to test the theoretical scaling behaviour as much as possible in order to see, whether the algorithms do what we think they should do.

We should try to find out what is the magnitude of reversibility violations in the HMC algorithm and attempt to quantify its impact on physical observables. If lack of reversibility appears to be a problem with the HMC method, one should use the multiboson technique or the Kramers equation algorithm.

Dynamical fermion simulations with Symanzik improved actions have already been started. Fig. 3 demonstrates that this can be done with only a small overhead for simulations that need more than about 250 iterations for the matrix inversion. If also for dynamical fermions improvement turns out to be important then this will lead to substantial progress in the area of fermion simulation algorithms.

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