Full QCD Algorithms towards the Chiral Limit

M. Hasenbusch [a]

[a]NIC/DESY Zeuthen, Platanenallee 6, D-15738 Zeuthen, Germany

I discuss the behaviour of algorithms for dynamical fermions as the sea-quark mass decreases. I focus on the Hybrid-Monte-Carlo (HMC) algorithm applied to two degenerate flavours of Wilson fermions. First, I briefly review the performance obtained in large scale HMC simulations. Then I discuss a modified pseudo-fermion action for the HMC simulation that has been introduced three years ago. I summarize recent results obtained with this pseudo-fermion action by the QCDSF and the ALPHA collaborations. I comment on alternatives to the HMC, like the Multiboson algorithm and variants of it.

1. INTRODUCTION

Today it is understood that further progress in the simulation of lattice QCD requires dynamical fermions. First large scale simulations with two flavours of degenerate Wilson fermions are done at a rather coarse lattice spacing $a \approx 0.1$ and are restricted to $m_{PS}/m_V > 0.5$. It is doubtful whether χ-perturbation theory can close the gap to the physical value $m_\pi/m_\rho \approx 0.18$ [1]. It seems that, for a given numerical effort, Kogut-Susskind (KS) fermions allow to reach smaller sea-quark masses than Wilson fermions [2]. For a critical review see [3]. Yet, biased by my personal experience, I shall restrict the following discussion to Wilson fermions. I expect that some statements also apply to KS fermions. To assess the progress that can be made with the machines of the near future, like QCDOC or apeNEXT, we have to understand the scaling of the algorithms at hand. Also it is clear that we should not only rely on the speed-up of computers but also should work on the simulation algorithms. Recent progress [4,5] with the Hybrid-Monte-Carlo (HMC) algorithm [6] and new ideas [7] presented earlier this year show that it is worth while to pursue this direction. For simplicity, we shall focus in the following on two degenerate flavours of sea-quarks. The corresponding partition function is given by $Z = \int \mathrm{D}[U] \quad \exp(-S_G[U]) \ \det M[U]^2$, where $S_G[U]$ is the gauge action and $M[U]$ the fermion matrix. For the definition see textbooks. Since the explicit calculation of the determinant of the fermion matrix is not feasible for reasonably large lattices, so called pseudo-fermion fields are introduced [8]:

$$\det M[U]^2 \propto \int \mathrm{D}[\phi] \int \mathrm{D}[\phi^\dagger] \exp(-S_{PF}[U,\phi,\phi^\dagger]) \ , \qquad (1)$$

where $S_{PF} = |M[U]^{-1}\phi|^2$ is the pseudo-fermion action. Since the inverse of the fermion matrix appears, the pseudo-fermion action S_{PF} is non-local and hence a local up-date of the gauge-field requires $O(Volume)$ operations, where $Volume$ is the number of sites of the lattice. It follows that a full sweep over the lattice costs $O(Volume^2)$ operations. To avoid this unfavourable scaling of the costs with the $Volume$, molecular dynamics evolution of the gauge field and eventually the HMC algorithm were introduced.

Later the multi-boson algorithm [9] was introduced. The inverse of the fermion matrix is approximated by some polynomial. This polynomial is factorized into its roots and for each factor, a boson-field is introduced. This way, the effective action becomes local. It can be simulated with a standard local Monte Carlo algorithm. However, it turned out that autocorrelation times increase considerably with increasing order of the polynomial.

2. THE HMC ALGORITHM

To allow the collective molecular dynamics evolution of the gauge-fields, new auxiliary variables, traceless Hermitian momenta $P_{x,\mu}$ conjugate to the gauge-field are introduced. The resulting effective Hamiltonian consists of the gauge action, the pseudo-fermion action and a new part for P: $H[U,\phi,\phi^\dagger,P] = S_G(U) + S_{PF}[U,\phi,\phi^\dagger] + \frac{1}{2}\sum_{x,\mu} \mathrm{Tr} P_{x,\mu}^2$. One elementary update ("trajectory") of the HMC algorithm is composed of the following steps:

a) Global heat-bath of the pseudo-fermions and the conjugate momenta.

b) Molecular dynamics evolution of the gauge-field U and the conjugate momenta P with fixed pseudo-fermions ϕ.

c) Accept/Reject step: the gauge-field U' that is generated by the molecular dynamics evolution is accepted with the probability $P_{acc} = \min[1, \exp(-H[U',\phi,\phi^\dagger,P'] + H(U,\phi,\phi^\dagger,P])]$, where P' represents the conjugate momenta generated in the molecular dynamics evolution.

The last step is needed, since the molecular dynamics evolution can not be done exactly and hence requires a numerical integration scheme, resulting in $\Delta H = H[U',\phi,\phi^\dagger,P'] - H(U,\phi,\phi^\dagger,P])] \neq 0$.

2.1. Integration Schemes

The HMC algorithm requires that the integration scheme used is area preserving and reversible. The simplest scheme that fulfills these requirements is the so called "leap-frog" algorithm. Let us define the update of the gauge-field and the momenta as

$$\begin{aligned} T_U(\delta\tau) &: \quad U \to e^{i\delta\tau\ P}\ U \\ T_P(\delta\tau) &: \quad P \to P - i\delta\tau\ \delta(S_g[U] + S_{PF}[U]) \ . \end{aligned}$$

Then, the elementary step of the leap-frog algorithm is given by

$$T_2(\delta\tau) = T_P\left(\frac{\delta\tau}{2}\right)\ T_U(\delta\tau)\ T_P\left(\frac{\delta\tau}{2}\right) \quad . \tag{2}$$

A trajectory is composed of N_{md} consecutive elementary steps. Its integration error is $O(\delta\tau^2)$ for a trajectory of a given length, where $\delta\tau$ is the step-size. Note that the order of the updates of momenta and gauge-fields is not unique. In fact, in ref. [19] it was demonstrated that the alternative order $T_2'(\delta\tau) = T_U\left(\frac{\delta\tau}{2}\right)\ T_P(\delta\tau)\ T_U\left(\frac{\delta\tau}{2}\right)$ achieves the same acceptance rate as eq. (2) (see fig. 2 of ref. [19]) with a roughly 15% larger step size $\delta\tau$. In the literature [10,11,12] also higher-order schemes are discussed. These schemes become increasingly complicated as the order increases. Recent studies, e.g. [13,14], with the standard pseudo-fermion action (1) show that higher-order schemes become less efficient than the simple leap-frog integration scheme as the sea-quark mass decreases.

Sexton and Weingarten [10] also suggested to split the update of the momenta into two parts:

$$\begin{aligned} T_{PG}(\delta\tau) &: \quad P \to P - i\delta\tau\ \delta_U S_g[U] \\ T_{PF}(\delta\tau) &: \quad P \to P - i\delta\tau\ \delta_U S_{PF}[U] \ . \end{aligned}$$

The leap-frog scheme is now generalized to

$$\begin{aligned} T_2(n,\delta\tau) \ &= \ T_{PF}\left(\frac{\delta\tau}{2}\right) \\ &\left[T_{PG}\left(\frac{\delta\tau}{2n}\right) T_U\left(\frac{\delta\tau}{n}\right) T_{PG}\left(\frac{\delta\tau}{2n}\right)\right]^n T_{PF}\left(\frac{\delta\tau}{2}\right) \end{aligned} \tag{3}$$

This allows to put a part of the action that is simple to compute (e.g. S_G) on a smaller time-scale than the rest.

2.2. Preconditioning

It has been noticed for a while that preconditioning of the fermion matrix is indispensable in lattice QCD simulations. First, the number of iterations needed to solve $M^{-1}\phi$ is reduced, but also the step-size of the HMC algorithm can be increased (See e.g. [15]). In addition to the even-odd preconditioning, SSOR preconditioning and variants of it [16] have been used in practice. The authors of ref. [17] have detailed how even-odd preconditioning can be applied to clover-improved Wilson fermions. They propose two possible variants. The asymmetric version:

$$\det M \propto \det(1_{ee} + T_{ee})\ \det\hat{M} \ , \tag{4}$$

where $\hat{M} = 1_{oo} + T_{oo} - H_{oe}(1_{ee} + T_{ee})^{-1} H_{eo}$. H_{oe} and H_{eo} is the hopping-matrix, connecting odd

with even sites and vice versa. T_{oo} and T_{ee} encode the clover term. The symmetric version is

$$\det M \propto \det(1_{ee}+T_{ee})\det(1_{oo}+T_{oo})\det\hat{M}_{sym} \ , (5)$$

where now $\hat{M}_{sym} = 1_{oo} - (1_{oo}+T_{oo})^{-1}M_{oe}(1_{ee}+T_{ee})^{-1}M_{eo}$. In most simulations, the asymmetric version (4) has been used. However, recently ref. [19] reported that the symmetric version (5) allows for a considerably larger step-size of the leap-frog than (4).

3. SCALING OF THE HMC

At the Lattice 2001 T. Lippert [18] reported about the scaling of the HMC algorithm based on the simulations of the SESAM collaboration. The result can be summarized as

$$N_{flops} = 2.3(7)\cdot 10^7 \cdot \left(\frac{L}{a}\right)^5 \cdot \left(\frac{1}{am_{PS}}\right)^{2.8(2)}$$

$$N_{flops} = 1.6(4)\cdot 10^7 \cdot \left(\frac{L}{a}\right)^5 \cdot \left(\frac{1}{am_{PS}}\right)^{4.3(2)}$$

for $\beta = 5.6$ and 5.5, respectively. The increase of the costs with decreasing mass m_{PS} of the pseudo-scalar meson has three sources:

a) Since the condition number of the fermion matrix increases as m_{PS} decreases, the solver needs more iterations to compute $M[U]^{-1}\phi$.
b) Decrease of the step-size $\delta\tau$ of the leap-frog integration scheme.
c) Increase of the autocorrelation time.

Here I like to briefly discuss the behaviour in two recent large scale simulations using clover-improved Wilson fermions. The CP-PACS collaboration [14] has simulated the Iwasaki gauge action at three β-values corresponding to the lattice spacings $a \approx 0.22, 0.16$ and 0.11 fm. The JLQCD collaboration [19] collaboration simulated the Wilson gauge action with $\beta = 5.2$ corresponding to $a \approx 0.09$ fm.

In table VI of ref. [14] integrated autocorrelation times for the plaquette, the number of iterations N_{inv} of the BiCGStab solver and the effective pion mass are given. Among these, τ_{Ninv} is the largest. For $\beta = 2.1$ ($a = 0.11$ fm) it behaves as $\tau_{Ninv} \propto (\kappa_c - \kappa)^{-0.3(2)}$. At the two smaller values of β, we see a slightly larger increase of the auto-correlation times, corresponding to the exponents $-0.5(1)$ and $-0.4(1)$. JLQCD [19] report autocorrelation times in table IV. In their case, the autocorrelation time of the plaquette even decreases as κ increases. Next, let us discuss the number of iterations required by the BiCGStab solver. The numbers for the $20^3 \times 48$ lattice given in table I of ref. [19] can be fitted as

$$N_{inv} = 0.253(4) \ (\kappa_c - \kappa)^{-0.893(2)} \ . \quad (6)$$

The numbers for N_{inv} given in table II of ref. [14] lead to virtually the same exponent. Fitting these numbers as a function function of m_{PS}, taken from table XXIII of ref. [14] gives $N_{inv} \propto m_{PS}^{-1.69}$. Finally, let us consider the step-size of the integration scheme. Taking the numbers for $\beta = 2.1$ from table II of ref. [14] for the step-size, we find $\delta\tau \propto (\kappa_c - \kappa)^{0.6}$. It is more difficult to extract such a result from the numbers of ref. [19], since the acceptance rate for the different values of κ vary quite a bit. Nevertheless it is clear from the numbers that the step-size has to be reduced considerably as κ increases. Taking into account the increase of N_{inv} and the decrease of $\delta\tau$ we get $cost \propto m_{PS}^{-z}$ with $z \approx 3$, which is similar to the results of ref. [18].

At the Lattice 2002, A. Irving [20] and Y. Namekawa [21] reported about explorative studies at light quark masses with $\frac{m_{PS}}{m_V} \approx 0.4$. Details of ref. [20] will be given below. In ref. [21] the Iwasaki gauge action at $\beta = 1.8$ ($a \approx 0.22$ fm) was studied at κ-values corresponding to $m_{PS}/m_V = 0.6$, 0.5 and 0.4. They find that the BiCGStab algorithm frequently fails to converge at the smaller quark masses. This problem was overcome by replacing the BiCGStab with the BiCGStab(DS-L) algorithm [22], which is a generalization of the BiCGStab. From fig. 2 of ref. [21] we see that a step size of $\delta\tau = 0.003$ had to be used at $m_{PS}/m_V \approx 0.5$ for a $12^3 \times 24$ lattice. Despite of this small step-size, spikes (i.e. extremely large ΔH) frequently occur (See fig. 2 of ref. [21]). They find that a reduction of the step-size $\delta\tau$ rapidly reduces the frequency of these spikes.

4. MODIFIED PSEUDO-FERMIONS

It has been observed by various authors that replacing the original fermion matrix by the even-odd preconditioned one allows for a larger step-size $\delta\tau$ in the HMC at constant acceptance rate. This lead to the idea [4] to factorized the fermion matrix such that each part has a smaller condition number than the original fermion matrix. In the modified pseudo-fermion action, for each of the factors a pseudo-fermion field is introduced. The splitting of the fermion matrix M can be written as $\bar{M} := W^{-1} M$. In ref. [4] W has been chosen as fermion matrix with a smaller hopping-parameter than M itself. Equivalently we get

$$W = M + \rho \ . \tag{7}$$

A second choice that we studied [23] is inspired by twisted mass QCD

$$W = M + i\rho\gamma_5 \ . \tag{8}$$

We introduce pseudo-fermions for both W and $\bar{M}$:

$$\begin{aligned} \det M M^\dagger \propto \int \mathcal{D}\phi_1^\dagger \int \mathcal{D}\phi_1 \int \mathcal{D}\phi_2^\dagger \int \mathcal{D}\phi_2 \\ \exp(-|W^{-1}\phi_1|^2 \ - |\bar{M}^{-1}\phi_2|^2) \end{aligned} \tag{9}$$

Hence, the modified pseudo-fermion action is then given by

$$S_F = S_{F1} + S_{F2} = |W^{-1}\phi_1|^2 \ + |\bar{M}^{-1}\phi_2|^2 \ . \tag{10}$$

For the practicability of the HMC algorithm it is important that the variation of S_F can be easily computed. For our choices of W, the variation of S_{F1} can be computed in the same way as the variation of S_F of eq. (1). Also the variation of S_{F2} can be explicitely computed: $\delta S_{F2} =$

$$X^\dagger \delta M Y - Y^\dagger \delta M^\dagger X + X^\dagger \delta W \phi_2 + \phi_2^\dagger \delta W^\dagger X \tag{11}$$

where $X = M^{\dagger -1} M^{-1} W \phi_2$, $Y = M^{-1} W \phi_2$. The experience with the 2D Schwinger model [4] has shown that the step-size of the integration scheme can indeed be increased by replacing the standard by the modified pseudo-fermion action. For the largest value of κ that we have studied, the step-size could be increased by a factor of two, while keeping the acceptance rate fixed. For a related approach see ref. [5].

4.1. Numerical results for Lattice QCD

Recently, detailed studies [23,24,25] of the modified pseudo-fermion action applied to the HMC simulation of Lattice QCD with two flavours of dynamical Wilson fermions have been carried out. In these studies, the method has been applied on top of even-odd preconditioning. I.e. the splitting is applied to $\hat{M}$. All three studies have used the asymmetric version (4) and (unfortunately) not eq. (5) as recommended by ref. [19]. The first question is, whether also here the step-size can be increased and how this scales with the sea-quark mass and the lattice size. In addition, it is important to check, whether there are effects of the modified pseudo-fermion action on the number of iterations needed by the solver, the autocorrelation times and the reversibility of the integration scheme.

In ref. [23] we simulated at $\beta = 5.2$ with $c_{sw} = 1.76$. Note that the final result of ref. [26] is $c_{sw} = 2.0171$. First we studied a $8^3 \times 24$ lattice at $\kappa = 0.137$. Later we simulated a $16^3 \times 24$ lattice at $\kappa = 0.139$, 0.1395 and 0.1398. Following ref. [27], these values of κ correspond to $m_{PS}/m_V \approx 0.856, 0.792, 0.715$ and 0.686, respectively.

We have tested two different integration schemes: The standard leap-frog and a partially improved one suggested by Sexton and Weingarten (see eq. (6.4) of ref. [10]) that has a reduced amplitude of the $O(\delta\tau^2)$ error compared with the leap-frog scheme. We used a trajectory length 1 throughout. To find the optimal value of the parameter ρ of the modified pseudo-fermion action, we have performed runs for different values of ρ with 100 trajectories each. For all these runs we used the same step-size $\delta\tau$. We looked for the value of ρ that gives the maximal acceptance rate. This search is not too difficult, since there seems to be only one local maximum, which is rather broad.

We have tested both splittings eq. (7) and eq. (8). We found a small advantage for eq. (7). A very important result is that the partially improved scheme gains more from the modified pseudo-fermion action than the leap-frog scheme. In particular for our smallest quark mass, given by $m_{PS}/m_V \approx 0.686$, the leap-frog performs better than the partially improved scheme in

the case of the standard pseudo-fermion action, while this order is just reversed when the modified pseudo-fermion action is used. In particular, we find for the $16^3 \times 24$ lattice with the standard pseudo-fermion action and the leap-frog scheme that $\delta\tau = 0.01$ is needed to get $P_{acc} = 0.77(3)$. With the modified pseudo-fermion action at the optimal ρ already $\delta\tau = 0.02$ gives $P_{acc} = 0.76(2)$. With the partially improved integration scheme and the standard pseudo-fermion action we get with $\delta\tau = 0.0166...$ an acceptance rate $P_{acc} = 0.82(2)$. The modified pseudo-fermion action with $\delta\tau = 0.066...$ gives $P_{acc} = 0.74(3)$. Comparing the two integration schemes, we have to note that for one elementary step, for the partially improved scheme, the variation of the force has to be computed twice as often as for the leap-frog. It remains an advantage of about $(0.066...)/(2 * 0.01) = 3.33...$ for the partially improved scheme combined with the modified pseudo-fermion action, compared with the leap-frog and the standard pseudo-fermion action. For a fair comparison, we also have to take into account the overhead caused by S_{F1} of the modified pseudo-fermion action. Taking the total number of iterations needed by the solver within one trajectory we arrive at a speed-up of $17000/6900 = 2.5$. Based on this experience it would be very interesting to study the behaviour of an $O(\delta\tau^4)$ improved integration scheme. Furthermore we find that reversibility violations are of similar magnitude for the modified pseudo-fermion action and the standard pseudo-fermion action. For the $8^3 \times 24$ lattice we performed extended runs with up to 8300 trajectories. From these runs we see that for the standard and the modified pseudo-fermion action as well as for different integration schemes, the autocorrelation times are the same, as long as the acceptance rate is the same.

The QCDSF collaboration [24] has simulated a $16^3 \times 32$ lattice at $\beta = 5.29$ with $c_{sw} = 1.9192$ and $\kappa = 0.1355$, which corresponds to $m_{PS}/m_V \approx 0.7$. Preliminary results for a $24^3 \times 48$ lattice at $\beta = 5.25$ with $c_{sw} = 1.9603$ and $\kappa = 0.13575$ are also available. This corresponds to $m_{PS}/m_V \approx 0.6$. They have used the pseudo-fermion action (7) and the leap-frog integration scheme with two time-scales (3). They compared three versions of the algorithm: (A) The HMC with the standard pseudo-fermion action, (B) the HMC with the modified pseudo-fermion action, where both S_{F1} and S_{F2} are on the same time-scale and (C) analogous to Sexton and Peardon [5], S_{F1} is on the same (smaller) time-scale as the gauge action. They have used a chronologicial prediction of the start vector for the solver.

For $m_{PS}/m_V \approx 0.7$ they find that (B) is about 2.8 times faster than (A). Similar to our experience [23], the step-size $\delta\tau$ of version (B) is twice the step size of (A). It is very surprising that an other factor of 1.4 speed-up comes from the iteration number of the solver. Naively one would expect that the larger step-size of version (B) would degrade the chronologicial prediction of the start vector and hence enlarge the iteration number. Maybe, with the modified pseudo-fermion action the evolution of the solution vector becomes smoother and hence the chronologicial prediction more effective. With version (C), they even find a speed-up of about 3.4 compared with (A). The preliminary results for $m_{PS}/m_V \approx 0.6$ are quite similar: with version (B) the speed-up is about 3.5 and with (C) 3.4. But here the parameters of the algorithm are not yet tuned much. Again the speed-up is partially due to a reduction of the iteration number of the solver in the case of (B) and (C) compared with (A).

The ALPHA collaboration [25] studied the pseudo-fermion action based on the splitting (8). They have used the partially improved integration scheme of Sexton and Weingarten. They imposed Schrödinger functional boundary conditions. They have studied lattices of size $L/a = 6$ up to $L/a = 24$ in a range $1.0 \leq u \leq 5.7$ of their renormalized coupling, corresponding to physical lattice sizes of 10^{-2} fm up to 1 fm. The range of β-values is $5.2 < \beta < 11.1$.

They have chosen the parameter ρ of the splitting following the rule $\rho \approx (< \lambda_{min} > / < \lambda_{max} >)^{1/4}$, where λ_{min} and λ_{max} are the minimal and maximal eigenvalues of $M^\dagger M$. The idea of this choice is that both $\bar{M}$ and W should have the same condition number. The runs where performed on a APEmille computer using single precision floating point numbers. Therefore spe-

cial attention on reversibility violations is needed. Their careful checks show that there is no relevant difference in this respect between the two pseudo-fermion actions. To check explicitly the effect of reversibility violations on the observables, they have varied the length of the trajectory. In addition to the usual $\tau = 1$ they studied $\tau = 0.5, 1.5$ and 3. They conclude that for $\tau = 1$, the reversibility violations do not invalidate the results of their simulations.

Since they performed rather long runs, even for $L/a = 24$ they have generated 4000 trajectories, they can give meaningful results for the autocorrelation times. Measured in units of trajectories, for the same acceptance rate, they find virtually no difference between the modified and standard pseudo-fermion action.

The main difference comes from the step-size that can be used to obtain an acceptance rate of about 80%. For the modified pseudo-fermion action, the step-size can be more than doubled compared with the standard case. There is only a rather small increase of this factor towards smaller values of β and larger L/a.

As a further test of the modified pseudo-fermion action, I have performed simulations at $m_{PS}/m_V \approx 0.4$ [28]. To this end I have taken the parameters reported by Irving at the Lattice 2002 [20]. He generated 2300 trajectories for a $16^3 \times 32$ lattice at $\beta = 5.2$, $c_{sw} = 2.0171$, $\kappa = 0.1358$. He obtained $m_{PS}/m_V = 0.43(2)$ and $m_\pi L = 3.3(1)$, where the last result indicates that the lattice size is actually too small to extract $L \to \infty$ results from the simulation. The result for the plaquette is $Plaq = 0.53770(4)$ with an autocorrelation time of $\tau \approx 7$. The step-size of the leap-frog scheme is $\delta\tau = 1/400$. The length of the trajectory is $\tau = 1$.

In my run I have tested only the modified pseudo-fermion action based on eq. (7). The partially improved integration scheme of Sexton and Weingarten is used. First I equilibrated the system for the parameters chosen. After some rough search for the optimal value of ρ, I generated 50 trajectories with 2 pseudo-fermion fields and the choice $\rho = 0.05$. With a step-size of $1/33$, $P_{acc} = 0.81(4)$ is obtained. Taking into account the fact that in the partially improved scheme the force has to be computed twice per step, we see a speed-up of $400/(2 \times 33) \approx 6$ compared with the run of Irving [20].

Then I simulated with 3 pseudo-fermion fields, i.e. splitting the fermion matrix into three factors. The parameters $\rho_1 = 0.4$ and $\rho_2 = 0.03$ of the corresponding pseudo-fermion action are guesses based on the experience with the two pseudo-fermion case. The fermion matrix is normalized such that it is 1 for $\kappa = 0$. After generating about 50 trajectories, we found that a larger step size than with two pseudo-fermions could be reached. Based on that we generated 1500 trajectories with a step-size of $\delta\tau = 1/25$. We find an acceptance rate of $P_{acc} = 0.809(6)$. The expectation value of the average plaquette is $Plaq = 0.53773(5)$, which is compatible with Irving's result [20]. The integrated auto-correlation time of the plaquette is $\tau = 7.5 \pm 3.0$. This again confirms that auto-correlation times depend very little on the pseudo-fermion action that is used.

In the simulation I have also seen a few spikes. The largest is $\Delta H \approx 3774$. The second largest is $\Delta H \approx 30$. These spikes are rather small compared with those of ref. [21] which are of order 10^5. Also $\langle \exp(-\Delta H) \rangle = 0.984(10)$ for my simulation seems to be fine. This result shows that the modified pseudo-fermion action not only allows for a larger step-size but also tames the spikes.

5. THE MULTIBOSON ALGORITHM

The qq+q collaboration has recently reported results for two-flavour Wilson simulations at quark masses in the range $\frac{1}{6}m_s < m_q < 2m_s$ using the TSMB version of the algorithm. A discussion of the performance, depending on the quark mass, the lattice size and the lattice spacing, is given in [29] (and refs. therein). The dependence on the pseudo scalar mass is given by $cost \propto m_{PS}^{-z}$ with $3 < z < 4$, which seems a little worse than the HMC algorithm. This is actually not too surprising. The increase of CPU cost with decreasing sea-quark mass in the MB algorithm and variants of it have mainly two sources: First the increase of the order of the polynomial and second the increase of autocorrelation times that are related to the order of the polynomial.

The increase of the order of the polynomial should be similar to the increase of the number of iteration of the solver in the HMC algorithm, which is the major source for the increasing effort in the HMC algorithm. On the other hand, for the MB algorithm, the numerical costs increase trivially with the lattice volume: $cost \propto (L/a)^4$, which compares favourably with the HMC algorithm, where we have $cost \propto (L/a)^5$ for the leap-frog integration scheme. The qualitative disadvantages of the MB algorithm compared with the HMC algorithm are the large memory requirement to store the boson-fields and the difficulty to implement the algorithm for improved fermion actions.

6. CONCLUSIONS

Tuned once more, the HMC algorithm seems to be a good choice for the simulation of dynamical Wilson fermions. One should take great care of all details like the precise choice of the integration scheme and the preconditioning of the fermion matrix. The modified pseudo-fermion action [4] speeds up the HMC simulation by allowing for a larger step-size of the integration scheme. Higher order integration schemes seem to profit more from the modified pseudo-fermion action than the leap-frog scheme. Hence, it seems likely that the scaling of the cost with the volume of the lattice can be improved to $cost \propto (L/a)^{4.5}$ by using an $O(\delta\tau^4)$ integration scheme, without negative side effects on the scaling with m_{PS}. The modified pseudo-fermion action introduces no unwanted side-effects like larger violations of reversibility or larger autocorrelation times. The proposal of Peardon [5] is more flexible than that of ref. [4]. Hence, it might lead to even larger speed-ups. Also it is straight forward to apply [5] to the Polynomial HMC algorithm. Whether new ideas [7] will beat the HMC remains to be seen.

REFERENCES

1. V. Bernard, S. Hashimoto, D.B. Leinweber, P. Lepage, E. Pallante, S. R. Sharpe and H. Wittig, Nucl. Phys. B (Proc.Suppl.) **119** (2003) 170, [hep-lat/0209086].
2. S. Gottlieb, Dynamical KS Fermion Result, these proceedings, [hep-lat/0310041]
3. K. Jansen, Dynamical Fermion Simulations, these proceedings.
4. M. Hasenbusch, Phys. Lett. B **519** (2001) 177, [hep-lat/0107019].
5. M. Peardon, Nucl. Phys. B (Proc.Suppl.) **106** (2002) 3, [hep-lat/0201003]; M. Peardon and J. Sexton, Nucl. Phys. B (Proc.Suppl.) **119** (2003) 985, [hep-lat/0209037].
6. S. Duane, A.D. Kennedy, B.J. Pendleton and D. Roweth, Phys. Lett. B **195** (1987) 216.
7. M. Lüscher, JHEP **0305** (2003) 052, [hep-lat/0304007].
8. D.H. Weingarten, D.N. Petcher Phys. Lett. B **99** (1981) 333.
9. M. Lüscher, Nucl. Phys. B **418** (1994) 637, [hep-lat/9311007].
10. J.C. Sexton and D.H. Weingarten, Nucl. Phys. B **380** (1992) 665.
11. M. Creutz and A. Gocksch, Phys. Rev. Lett. **63** (1989) 9.
12. M. Campostrini and P. Rossi, Nucl. Phys. B **329** (1990) 753.
13. T. Takaishi, Comput. Phys. Commun. **133** (2000) 6, [hep-lat/9909134].
14. S. Aoki et al., CP-PACS collaboration, Phys. Rev. D **65** (2002) 054505, [hep-lat/0206009].
15. R. Frezzotti, M. Hasenbusch, J. Heitger, K. Jansen and U. Wolff, Comput. Phys. Commun. **136** (2001) 1, [hep-lat/0009027].
16. S. Fischer, A. Frommer, U. Glaessner, Th. Lippert, G. Ritzenhoefer and K. Schilling, Comput. Phys. Commun. **98** (1996) 20, [hep-lat/9602019].
17. K. Jansen and C. Liu, Comp. Phys. Commun. **99** (1997) 221, [hep-lat/9603008].
18. T. Lippert, Nucl. Phys. B (Proc.Suppl.) **106** (2002) 193, [hep-lat/0203009].
19. S. Aoki et al., JLQCD collaboration, hep-lat/0212039, to be published in Phys. Rev. D.
20. A.C. Irving, UKQCD collaboration, hep-lat/0208065, Nucl. Phys. B (Proc.Suppl.) **106** (2002) 341.
21. Y. Namekawa et al., CP-PACS, Nucl. Phys. B (Proc. Suppl.) **106** (2002) 335,

[hep-lat/0209073].
22. G.L.G. Sleijpen and D.R. Fokkema, Elec. Trans. on Numer. Anal. Vol.1 (1993) 11; T. Miyauchi et al., Trans. of Japan Soc. for Ind. and Appl. Math. Vol. 11, No.2 (2001) 49.
23. M. Hasenbusch and K. Jansen, Nucl. Phys. B **659** (2003) 299, [hep-lat/0211042].
24. QCDSF collaboration, A. Ali Khan et al., hep-lat/0303026, Phys. Lett. B **564** (2003) 235; A. Ali Khan et al., these proceedings, [hep-lat/0309078].
25. ALPHA collaboration, M. Della Morte et al., hep-lat/0307008, M. Della Morte et al., these proceedings, [hep-lat/0309074].
26. K. Jansen and R. Sommer, Nucl. Phys. B **530** (1998) 185, [hep-lat/9803017].
27. Z. Sroczynski, Ph.D. thesis, Edinburgh (1998).
28. M. Hasenbusch, to be published.
29. I. Montvay, hep-lat/0301013, to appear in the Proceedings of SEWM, Heidelberg, (2002).