Experiences with the
Polynomial Hybrid Monte Carlo Algorithm [*]

Roberto Frezzotti

DESY

Notkestr. 85

D-22603 Hamburg, Germany

Karl Jansen

CERN 1211 Genève 23

Switzerland

Abstract

We discuss a simulation algorithm for dynamical fermions, which combines the multi-boson technique with the Hybrid Monte Carlo algorithm. The algorithm turns out to give a substantial gain over standard methods in practical simulations and to be suitable for dealing with fermion zero modes in a clean and controllable way.

1 Introduction

In this contribution, we discuss a simulation algorithm, which we call Polynomial Hybrid Monte Carlo (PHMC) [1], for full lattice QCD, implemented in the case of Wilson fermions. The algorithm is based on two key ingredients, the interplay of which appears to be crucial for a performance gain over the standard HMC algorithm. The generation of gauge-field configurations

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is performed as first proposed in [2]: the usual inverse of the Dirac operator is approximated (as in Lüscher's multiboson algorithm [3]) by a polynomial in the operator and, with this polynomial defining the fermion action, the simulation is done using a standard small-step Monte Carlo method. The second crucial ingredient is the way of correcting for the above-mentioned polynomial approximation. We suggest to do this by means of an efficient reweighing technique, which is reminescent of earlier ideas, such as [4], and allows us to deal in a clean and controllable way with fermion zero modes, as discussed below.

2 The PHMC algorithm

Denoting by U the configuration of lattice gauge links, the expectation value of any gauge invariant observable $\mathcal{O} = \mathcal{O}[U]$, in full QCD with $n_f = 2$ degenerate flavours, may be written as

$$\langle \mathcal{O} \rangle = \mathcal{Z}^{-1} \left[\int \mathcal{D}U e^{-S_g[U]} \det(Q^2[U]) \mathcal{O}[U] \right] , \tag{1}$$

where S_g is the standard plaquette action for the pure gauge sector $(\beta = 6/g_0^2)$ and Q is the Dirac operator for Wilson fermions multiplied by γ_5:

$$Q[U]_{x,y} = c_0 \gamma_5 \left[\left(1 + \frac{i}{2} \kappa c_{SW} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right) \delta_{x,y} \right.$$
$$\left. -\kappa \sum_\mu P_\mu^- U_{x,\mu} \delta_{x+\mu,y} + P_\mu^+ U_{x-\mu,\mu}^\dagger \delta_{x-\mu,y} \right] \tag{2}$$

with $P_\mu^\pm = 1 \pm \gamma_\mu$, $\hat{F}_{\mu\nu}$ the standard 'clover' discretization of $F_{\mu\nu}$, and $Q^\dagger = Q$. Here we present simulation results only for $c_{SW} = 0$. For $c_{SW} > 0$ the computational cost per single molecular dynamics trajectory has been evaluated and performance tests are in progress.

We use the polynomial approximation of $(Q^2)^{-1}$ described in [4]: the polynomial of degree n, denoted as $P_{n,\epsilon}(s)$, approximates s^{-1} in the range $\epsilon < s < 1$ with a relative fit error bounded by $\delta = 2 \left(\frac{1-\sqrt{\epsilon}}{1+\sqrt{\epsilon}} \right)^{n+1}$ (where $\epsilon > 0$). Choosing c_0 such that $\|Q^2\| < 1$, we may write the corresponding polynomial of Q^2 in a factorized form:

$$P_{n,\epsilon}(Q^2) = C_{n,\epsilon} \prod_{k=1}^n (Q - r_k^*)(Q - r_k) , \tag{3}$$

where $C_{n,\epsilon}$ is a positive constant, $r_k \equiv \sqrt{z_k} = \mu_k + i\nu_k$ and the z_k's are the complex roots of $P_{n,\epsilon}(s)$, as in [4]. For the values of n and ϵ used in our tests, a careful ordering of the monomial factors appearing in (3) was essential, at least on computers with 32-bit precision, in order to keep to a negligible level the rounding error in constructing $P_{n,\epsilon}(Q^2)$ using the factorized form, eq.(3).

The full QCD $(n_f = 2)$ partition function may be represented as

$$\mathcal{Z} = \int \mathcal{D}U \mathcal{D}\phi^\dagger \mathcal{D}\phi \mathcal{D}\eta^\dagger \mathcal{D}\eta W e^{-(S_g + S_P)}$$
$$S_P = S_P[U, \phi, \eta] = \phi^\dagger P_{n,\epsilon}(Q^2[U])\phi + \eta^\dagger \eta \tag{4}$$

by introducing the auxiliary pseudofermion fields (i.e. boson fields with spin and colour indices) ϕ, η and the 'correction' factor $W = W[\eta, U]$:

$$W = \exp\left\{\eta^\dagger(1 - [Q^2 \cdot P_{n,\epsilon}(Q^2)]^{-1})\eta\right\} . \tag{5}$$

In the PHMC algorithm, the update of the gauge field configuration is performed by using the Φ-version [5] of the HMC algorithm for the 'approximate' but still non-local action $S_g + S_P$ of eq. (4). We denote averages in the theory with action $S_g + S_P$ as $\langle\ldots\rangle_P$: reweighing with W yields the true averages, denoted as $\langle\ldots\rangle$, for any observable $\mathcal{O} = \mathcal{O}[U]$:

$$\langle\mathcal{O}\rangle = \langle W\rangle_P^{-1}\langle\mathcal{O}W\rangle_P . \tag{6}$$

The number (N_{corr}) of evaluations of W per single molecular dynamics trajectory (updating U) is relevant for the level of statistical error on $\langle\mathcal{O}\rangle$, although $\langle\mathcal{O}\rangle$ itself is correct, within statistical uncertainties, for any value of N_{corr}. Each evaluation of W requires a trivial Gaussian update of the η-field and the solution of the system $[Q^2 P_{n,\epsilon}(Q^2)]\chi = \eta$.

3 The results

All the results discussed here, for both HMC and PHMC algorithms, have been obtained using the even-odd preconditioned form of the Q operator, denoted by $\hat{Q}$, and a Sexton-Weingarten leap-frog integration scheme. We adopted Schrödinger functional boundary conditions and monitored few observables: the plaquette (P), the lowest (λ_{min}) and the highest (λ_{max}) eigenvalues of $\hat{Q}^2$ (normalized in such a way that $\lambda_{max} \lesssim 1$).

Several tests on the 4^4 lattice with different values of (n, ϵ) showed that the chosen polynomial approximation should not be too bad, in order to avoid that reweighing observables with W induce large statistical fluctuations in true averages. The approximation should not be too good either, in order to keep as low as possible the computational cost per single trajectory (of length $\simeq 1$). In practice, a reasonable compromise is obtained by choosing $\epsilon \simeq 2\langle\lambda_{min}\rangle$ and n such that $\delta \simeq 0.01$–0.02, which means n scaling as $\epsilon^{-1/2}$. This criterion (plus short runs monitoring the statistical fluctuations of W) allows us to quickly choose reasonable values of (n, ϵ).

In Table 1, we compare HMC and PHMC algorithms, as far as the computational cost per single trajectory and the relative statistical error for P and λ_{min} are concerned. Bare lattice parameters are $\beta = 6.4$, $\kappa = 0.15$ on the 4^4 lattice. On the 8^4 lattice we choose $\beta = 5.6$ and $\kappa = 0.1585 \simeq \kappa_c$, which are the same bare parameters used for comparing the multiboson technique and the HMC algorithm in ref. [6]. The chosen values of (n, ϵ, N_{corr}) are $(12, 0.036, 1)$ for the 4^4 lattice, corresponding to one of the best choices, and $(48, 0.026, 2)$ for the 8^4 lattice. The values of ϵ reflect a factor larger than 10 for the condition number of $\hat{Q}^2$, between the 8^4 and 4^4 lattices. Further details concerning the results reported in Table 1, such as the proper definition of the computational costs, molecular dynamics parameters

L^4	Algorithm	$C_{Q\phi}$	$\sigma(P)/\langle P \rangle$	$\sigma(\lambda_{min})/\langle \lambda_{min} \rangle$
4^4	PHMC	540	0.00024	0.0064
4^4	HMC	868	0.00020	0.0057
8^4	PHMC	3974	0.00027	0.037
8^4	HMC	7398	0.00021	0.039

Table 1: We give the single trajectory cost, $C_{Q\phi}$, in units of $Q\phi$ operations. We compare the relative statistical errors for P and λ_{min}, obtained from a jack-knife blocking analysis, with 18000 and 2745 trajectories for 4^4 and 8^4 lattices, respectively. Note that we estimate a 10 to 20% uncertainty on the statistical errors.

and average values with statistical uncertainties, may be found in ref. [1]. The formulae for computational costs appearing there are also valid for the O(a)-improved fermions ($c_{SW} > 0$).

Looking mainly at the 8^4 lattice case, which is the one with a relatively large condition number of about 700, our results for the PHMC algorithm may be summarized as follows. First, average values of measured observables always agree with the corresponding ones from the HMC algorithm (within statistical uncertainties); without reweighing with W, systematic deviations, increasing with $1 - \langle W \rangle_P$, are observed, as expected. Second, for suitable choices of (n, ϵ), the statistical errors of measured observables are the same as for the HMC algorithm, at least within their relative uncertainty, which we estimate to be about 10–20%. At the same time, the computational cost per single trajectory, $C_{Q\phi}$, is almost a factor of 2 lower than for the HMC algorithm. This is a consequence of the fact that $C_{Q\phi}$ is basically proportional to ϵ^{-1} for the PHMC and to λ_{min}^{-1} for the HMC algorithm. Last but not least, we find that PHMC and HMC algorithms sample configuration space in a somewhat different way: for instance, the low-lying end of the distributions of λ_{min} look different (Fig. 1).

As expected from the properties of the polynomial approximation of $(\hat{Q}^2)^{-1}$, the PHMC algorithm generates configurations with low-lying modes ($\lambda_{min} < \epsilon$) of $(\hat{Q}^2)$ with a higher probability than algorithms like HMC or the multiboson technique made exact by an accept/reject step [7]: in particular the PHMC algorithm generates, with small, non-zero probability, configurations carrying fermion zero modes, which occur with vanishing probability (i.e. never in a finite run time) when using the other algorithms mentioned above. However, fermion zero modes give a finite, non-zero contribution to all those observables where the divergence of quark propagators compensates for the vanishing of the probability measure. In ref. [1], we discuss how we may in principle deal with fermion zero modes, in order to evaluate the correction factor W and quark propagators, by making use of existing minimization algorithms (tested up to $\lambda_{min} \sim 10^{-18}\lambda_{max}$). Therefore, the PHMC algorithm looks particularly suitable to study the contribution of low-lying fermion modes to physical observables in full QCD. For the same reasons, one may also expect that the PHMC algorithm may overcome energy barriers, related to low-lying fermion modes, easier than the HMC algorithm, leading to a better exploration of
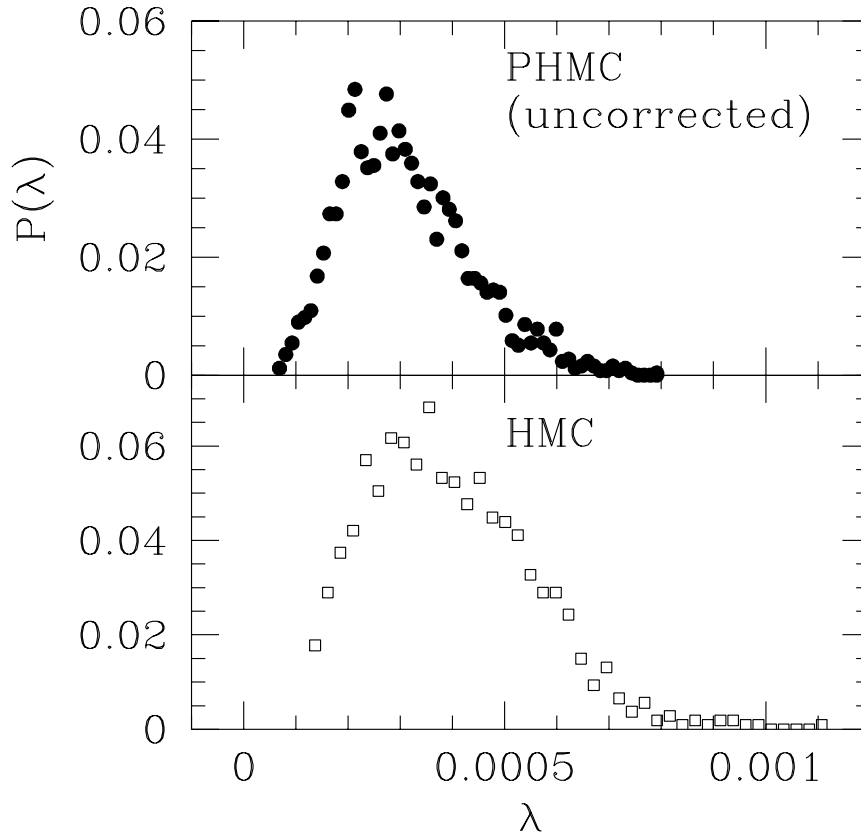
Figure 1: The distribution of $\lambda = \lambda_{min}(\hat{Q}^2)$ as obtained with equal statistics on the 8^4 lattice for both PHMC and HMC algorithms.

configuration space.

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