Local bosonic versus HMC — a CPU cost comparison

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We compare the CPU cost of HMC to various implementations of the Hermitean variant of Lüscher’s local bosonic algorithm (LBA) for 2D massive QED with two flavours of Wilson fermions. We carefully scan a 3-dimensional parameter subspace and find flat behaviour around the optimum. The gain factor of the LBA, as compared to HMC, is slightly smaller for the Re-weighting method than for the Metropolis variants and estimated to about 3.3 for the plaquette and 1.9 for the the meson correlator.

1. Schwinger model

For our tests we select as a low-cost laboratory the massive 2-flavour Schwinger model (2D QED) \cite{1}. The lattice model is given by the Wilson plaquette and fermionic action. For details we refer to last year’s proceedings \cite{2}. We work with the Hermitian fermion matrix \( Q = cγ_5 M \) scaled so that its eigenvalues are in \([-1, 1]\).

2. Hybrid Monte Carlo

To set the scale, we simulate using a HMC code working also with the Hermitian matrix \( Q \). The implementation includes optimization features like trajectory length set by \( n \cdot Δτ = 1 \) and acceptance \( ≈ \) 70%, and re-use of the CG solution in the trajectory via \( \bar{x} = 0 \) (gain \( ≈ 20\%) \).

3. Hermitean local bosonic algorithm

Alternatively to HMC, M. Lüscher proposed a local bosonic formulation \cite{3}. The one main variant we consider uses the fact that we are dealing with a Hermitian fermion matrix thus allowing to exactly rewrite the effective distribution

\[
P_{eff} \propto \det Q^2 e^{-S_p(U)} \propto \det(1-R) \det(P_n(Q^2)^{-1}) e^{-S_p(U)}
\]

with \( P_n(s) \) a polynomial of even degree \( n \) approximating \( \frac{1}{s} \) for real \( s \in [ε, 1] \) such that the correction factor \( \det(1-R) = \det(Q^2P_n(Q^2)) \approx 1 \). Its roots \( z_k (k = 1...n) \) come in complex conjugate pairs and determine \( \sqrt{z_k} = μ_k + iν_k \ (ν_k > 0) \). This leads to a totally bosonic representation

\[
P_{eff} \propto \det[1-R]e^{-S_p(U)} \int Dφ e^{-\sum_k φ_k^2[(Q-μ_k)^2+ν_k^2]}φ_k
\]

with \( n \) complex bosonic Dirac fields \( φ_k \). We chose as approximation polynomials \( P_n(s) \) the Chebyshev polynomials proposed by Bunk et al.\cite{4}. The convergence of \( P_n(s) \rightarrow 1/s \) as \( n \rightarrow ∞ \) is exponential and uniform for \( s \in [ε, 1] \). One update of the bosonic system consists of a trajectory of heat bath and over-relaxation steps for \( U \) and \( φ \) fields, possibly followed by a Metropolis acceptance correction for \( det[1-R] \). In total, this introduces the parameters \( n, ε \) and the number of reflections per heat bath into the algorithm.

4. Exact algorithm

The correction factor can be treated exactly with a Metropolis accept/reject step or Re-weighting\cite{5} using a stochastic method as demonstrated for the non-Hermitean variant \cite{6}.

The Re-weighting method computes a noisy estimate for \( det[1-R] \) and includes it in the observables.

The Metropolis correction step uses an acceptance probability \( P^A(χ) \) dependent on a Gaussian noise \( χ \) which satisfies detailed balance when averaged over the noise. This can be achieved formally by

\[
P^A_{U,φ→U',φ'} = \min(1, e^{-χ^T[1-R']^{-1}Bχ+χ^Tχ})
\]
with $B$ given by $BB^\dagger = Q^2 P_n(Q^2)$. In the Hermitean case this is non-trivial to solve. The task becomes trivial, if we recall the factorized form

$$Q^2 P_n(Q^2) = Q^1 Q_{\text{norm}} \prod_k (Q^2 - z_k)(Q^2 - \bar{z}_k)$$

taking one factor from each c.c. pair.

We remark that the Metropolis scheme includes a further optimization possibility which we call Metropolis with adapted precision. We retain a valid algorithm if the inversion necessary for the Metropolis decision is first executed with very small precision (in our case $\delta = 10^{-2}$) and repeated with standard inverter precision ($\delta = 10^{-6}$) only if the decision would else be unclear. As the CG can be restarted from the intermediate solution, this procedure could result in less work on the average.

5. Numerical instabilities

Evaluating a high order polynomial for a matrix faces the problem of loss of precision. In the non-Hermitean variant or Re-weighting case we are able to avoid this by using the Chebyshev recursion formula for $R$. Unfortunately the Hermitean variant with Metropolis correction or the Polynomial Hybrid Monte-Carlo algorithm [9] rely on the evaluation of partial products of root factors.

In a forthcoming publication [10], we compare various proposals for reordering the roots to minimize numerical instabilities. In this work, we use a fairly stable version, the so-called Bitreversal scheme, whenever no recursion is possible.

Recently, one of us proposed a different solution [11]. We rewrite the Metropolis acceptance to

$$P_{U \phi \rightarrow U' \phi'} = \min \left(1, e^{\eta(R - R')} \right),$$

with $\eta$ given by $\chi = |Q^2 P_n(Q^2)|^2 \eta$. At this point we suggest solving for the inverse of the square root of $Q^2 P_n(Q^2)$ directly. This can be accomplished with an expansion in Gegenbauer polynomials converging exponentially with the same rate as CG.

6. Observables – $\kappa$ value

We simulate on 8x20 lattices with a conservative $\beta = 3.0$ and a run length of usually $>1000\tau$, calculating the plaquette and correlations of local meson operators $\langle \bar{\Psi} \gamma^5 \Psi \rangle (\pi)$, $\langle \bar{\Psi} \gamma^5 \Psi \rangle (a_0)$, $\langle \bar{\Psi} \gamma^5 \Psi \rangle (\eta).$ We expect finite size effects to appear in deviations from the approximately linear behaviour of the pion mass with $\kappa$. As shown in Fig. 6 finite size effects are small for $\kappa \leq 0.24$, resulting in a pion mass $m_\pi = 0.629$ and a physical ratio $m_\pi/m_\eta = 0.807$.

7. Cost comparison

To summarize, we repeat the schemes included in our investigation. Besides Hybrid MC to set the scale, we compare LBA with Re-weighting, LBA with Metropolis, and LBA with Metropolis using adapted precision, and LBA with Gegenbauer inverter as described above.

We point out that Re-weighting and Metropolis algorithms result in 2 different ensembles. Therefore it is no longer possible to compare CPU cost by

$$C = \frac{2\tau_{\text{int}}}{N_{\text{meas}}} \cdot N_{\text{all Q ops}}$$

but one has to use a measure based on the relative error

$$C_{\text{eff}} = N_{\text{all Q ops}} \cdot \frac{\sigma^2_{\text{tot}}(A)}{A^2}.$$
Figure 2.

Cost for Plaquette (opt # relexions) -- Metropolis

| n | epsilon |
|---|---------|
| 5 | 10      |
| 10| 20      |
| 15| 25      |
| 20| 30      |
| 25| 35      |
| 30| 40      |

Table 1
CPU cost minima - Plaquette

| algorithm            | n  | epsilon | refl. | cost | gain |
|----------------------|----|---------|-------|------|------|
| HMC                  |    |         |       | 6.1  |      |
| Metro 1              | 18 | 0.02    | 2     | 1.9  | 3.3  |
| Metro 2              | 18 | 0.02    | 3     | 2.1  | 2.9  |
| Gegenbauer           | 18 | 0.01    | 2     | 2.0  | 3.0  |
| Re-weighting         | 24 | 0.02    | 4     | 2.6  | 2.4  |

In these formulae $N_{\text{meas}}$ signifies the number of measurements, $N_{\text{all Q ops}}$ the total number of matrix multiplications for the whole run.

To illustrate our search for optimal parameters, we depict in Fig. 2 the CPU cost in the $n - \epsilon$ plane (number of reflections optimized) for one algorithm, namely plain Metropolis. The figure clearly shows that we obtain a flat optimum.

We further compare only the optimal parameter sets and their CPU cost in table 1.

8. Conclusions

We think that this study gives further clear evidence that the LBA is competitive to HMC. The tuning of the LBA is fairly easy. The CPU cost can be lower than for HMC, but not by a large factor with present techniques. We want to stress that the gain factors for the plaquette and pion propagator differ with estimates from plaquette-like observables too optimistic.

Technically, the number of reflections per heat-bath update is found to be an important optimization tool. We also demonstrate that using a Noisy Metropolis scheme to make the LBA exact is possible for the Hermitean case as well. The Gegenbauer inverter, which avoids instabilities in the evaluation of the polynomial, is shown to be competitive to CG in a first real simulation.

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