Comparing iterative methods for overlap and twisted mass fermions

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We present a systematic comparison of various iterative methods to obtain the fermion propagator with both overlap and twisted mass fermions at fixed pion mass in the quenched approximation. Taking the best available algorithm in each case we find that calculations with the overlap operator are by a factor of 20-40 more expensive than with the twisted mass operator at the parameter values considered here. For the overlap operator we also compare the efficiency of various methods for calculating the topological index.

1. INTRODUCTION

The Wilson twisted mass (Wtm) lattice fermion action of an SU_{f}(2) flavour doublet of mass degenerate quarks with maximal twist angle has the form

\[ D_{\text{tm}}(\mu) = D_{\text{w}}(m_{\text{tm}}) + i\gamma_{5}\tau_{3} \cdot \mu \]

where \( D_{\text{w}} \) is the Wilson Dirac operator, \( m_{\text{tm}} \) the bare quark mass tuned to its critical value and \( \mu \) the twisted quark mass. For our purpose it is sufficient to consider only one of the two flavours.

The massive overlap operator is defined as

\[ D(m_{\text{ov}}) = \left( 1 - \frac{m_{\text{ov}}}{2\rho} \right) D + m_{\text{ov}} \]

where

\[ D = \rho \left( 1 + \gamma_{5} \text{sign}(Q(\rho)) \right) \]

is the massless overlap operator with \( Q(\rho) = \gamma_{5}D_{W}(-\rho) \), \( \rho = 1.6 \) and \( m_{\text{ov}} \) the bare quark mass.

For both Wtm and the overlap operator we present results using the inversion algorithms GMRES(m), CG(NE), CGS and BiCGstab [1] and additionally MR [1] and SUMR [2,3] for the overlap operator.

2. SETUP

Our set-up consists of two quenched ensembles of 20 lattices with \( V = 12^{4} \) and \( 16^{4} \) each generated with the Wilson gauge action at \( \beta = 5.85 \) corresponding to a lattice spacing of \( a \sim 0.12 \) fm.

We invert both the twisted mass and the overlap operator on two point-like sources \( \eta \) with two different bare quark masses and require a stopping criterion \( |Ax - \eta|^{2} < 10^{-14} \).

The quark masses \( m_{\text{ov}} = 0.10 \) and \( m_{\text{ov}} = 0.03 \) for the overlap and \( \mu = 0.042 \) and \( \mu = 0.0125 \) for the twisted mass are chosen such that the corresponding pion mass for the twisted mass and the overlap operator are matched:

\[ m_{\pi} = 720 \text{MeV} \Rightarrow \begin{cases} m_{\text{ov}} = 0.10 \\ \mu = 0.042 \end{cases} \]

\[ m_{\pi} = 390 \text{MeV} \Rightarrow \begin{cases} m_{\text{ov}} = 0.03 \\ \mu = 0.0125 \end{cases} \]

We are working in a chiral basis and the two sources are chosen so that they correspond to sources in the two different chiral sectors. For the CG(NE) algorithm using the overlap operator we can then use the relation

\[ P_{\pm} D(m_{\text{ov}}) D(m_{\text{ov}}) P_{\pm} = 2P_{\pm} D(m_{\text{ov}}^{2}/(2\rho)) P_{\pm} \]

where \( P_{\pm} \) are the chiral projectors, since the inversions take place in a given chiral sector. This saves a factor of two with respect to the general
CG(NE) case and in the following we denote this algorithm by CG$_\chi$.

The computational bottleneck for the inversions of the overlap operator is the computation of the approximation of the sign-function sign($Q$). Our approximations use Chebyshev polynomials of the order $O(200-300)$. In order to achieve this we project out the lowest 20 and 40 eigenvectors of the hermitian Wilson Dirac operator $Q(\rho)$ on the $12^4$ and $16^4$ lattice, respectively.

It is well known that by adapting the accuracy of the approximation during the course of the iteration one can speed up the inversions by large factors since a reduction in the order of the polynomial enters multiplicatively in the total cost of the inversion. In the following we denote these algorithms by the subscript $\text{ap}$ for adaptive precision. The precision is adapted so as to ensure that no contributions to the sign-function approximation are calculated which are not needed at the present stage of the algorithm. In the case of the CG$_{\text{ap}}$ we simply calculate contributions up to the point where they are smaller by a factor $O(10^{-2})$ than the desired residuum. This requires the full polynomial only at the beginning of the CG-search while towards the end of the search we use polynomials of the order $O(10)$. In the case of MR$_{\text{ap}}$, we start with a low order approximation of $O(10)$ right from the beginning. Subsequently the introduced error is corrected from time to time by calculating the true residuum to full precision.

<table>
<thead>
<tr>
<th>$V$, $m_\pi$</th>
<th>Overlap</th>
<th>Wtm</th>
<th>rel. factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$12^4$, 720Mev</td>
<td>48.8(6)</td>
<td>2.6(1)</td>
<td>18.8</td>
</tr>
<tr>
<td>$12^4$, 390Mev</td>
<td>142(2)</td>
<td>4.0(1)</td>
<td>35.4</td>
</tr>
<tr>
<td>$16^4$, 720Mev</td>
<td>225(2)</td>
<td>9.0(2)</td>
<td>25.0</td>
</tr>
<tr>
<td>$16^4$, 390Mev</td>
<td>653(6)</td>
<td>17.5(6)</td>
<td>37.3</td>
</tr>
</tbody>
</table>

Table 1
Best absolute timings in seconds.

3. RESULTS

We first present the relative timings of the algorithms for both the overlap and twisted mass operators in Figure 1 where in each case the timings are relative to the fastest algorithm. The timings were all obtained on one node of the Juelich Multiprocessor (JUMP) IBM p690 Regatta using 32 processors.

Next we compare directly the absolute and relative cost for the overlap and twisted mass operator in Table 1 where we pick in each case the best available algorithm, GMRES$_{\text{ap}}$ for the overlap and CGS for twisted mass.

4. TOPOLOGICAL CHARGE COMPUTATION

For the computation of the topological index it is important to note that the determination of the chiral sector which contains the zero-modes comes for free when one uses the CG-algorithm for the inversion. From the CG-coefficients which are obtained during the iteration one can build up a tridiagonal matrix related to the underlying Lanczos procedure. The eigenvalues of this matrix approximate the extremal eigenvalues of the operator and it turns out that the lowest 5-10 eigenvalues are approximated rather accurately. By estimating the eigenvalues once in each chiral sector and by pairing them accordingly it is possible to identify the chiral sector which contains zero modes.

In order to determine the topological charge itself one has to compute the lowest eigenvalues of the overlap operator as well as their degeneracies. We have implemented two different algorithms, one based on the Ritz-Jacobi (RJ) method and the other based on the Jacobs-Davidson (JD) method. Both of them are improved by looking separately in the two chiral sectors using adaptive precision.

We compare the two algorithms on a $12^3 \times 24$ and a $16^4$ lattice at $\beta = 5.85$ and $\rho = 1.6$ with five configurations each. Both methods first determine the chiral sector containing zero modes and subsequently all the zero modes are calculated in this sector. With the JD method additionally two non zero modes have been computed. The timings relative to RJ are 0.73(9) on the $12^3 \times 24$ lattice and 0.93(7) on the $16^4$ lattice.

The performance of both methods is compa-
Figure 1. Relative timings of the various algorithms for the overlap (left column) and the twisted mass operator (right column).

5. CONCLUSIONS AND OUTLOOK

We find that for Wtm fermions CGS appears to be the fastest inversion algorithm while for overlap fermions it is GMRES$_{ap}$ for the parameters investigated here. In a direct competition between twisted mass and overlap fermions the latter are by a factor of 20-40 more expensive if one compares the best available algorithms in each case.

For the index computation a clever combination of the methods described above looks most promising. Finally we note that one can apply various kinds of preconditioning to all the algorithms investigated here. For the twisted mass operator low-mode preconditioning should be very effective for low quark masses.

REFERENCES