Improving Inversions of the Overlap Operator

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We present relaxation and preconditioning techniques which accelerate the inversion of the overlap operator by a factor of four on small lattices, with larger gains as the lattice size increases. These improvements can be used in both propagator calculations and dynamical simulations.

1. INTRODUCTION

The massive overlap operator can be written as

\[ D_u = \rho I + \gamma_5 \text{sign}(Q), \]

where \( \rho \geq 1 \) is a mass parameter corresponding to a bare fermion mass \( m_b = m(\rho - 1) \), and \( Q \) is the hermitian Wilson operator with a negative mass parameter \( -m \). Note that \( \gamma_5 \text{sign}(Q) \) is unitary. We can also define a hermitian overlap operator \( D_h = \gamma_5 D_u \). Both operators are normal, i.e. they commute with their adjoints. We will approximate the matrix sign function using the Zolotarev partial fraction expansion (ZPFE),

\[ \text{sign}(Q) = \sum_{i=1}^{N_Z} \omega_i Q = \sum_{i=1}^{N_Z} \frac{\omega_i Q}{Q^2 + \tau_i}, \]

where the coefficients \( \omega_i \) and \( \tau_i \) are known \cite{1}, and the accuracy of the approximation depends on the Zolotarev order \( N_Z \). Multiplication of the ZPFE with a vector is easily implemented using a multishift CG-inversion \cite{2}.

In these proceedings, we will sketch how to optimise the inversion of \( D_u \) (the propagator calculation), and \( D_h^2 \) (the full inversion). Both these inversions can be reduced to solving for the vector \( x \) in any of the three following equations:

\[ D_u x = b, \quad D_h x = \gamma_5 b, \quad D_h D_h x = b. \]

2. SUMR

The optimal method to solve equation (2) is well known to be the minimal residual (MINRES). Similarly, for equation (3) the conjugate gradient (CG) method is optimal. Less well known is the shifted unitary minimal residual (SUMR) method \cite{3,4}, which can be used to invert equation (1). There are known formulae for the accuracy of the inversion for each of these methods after \( k \) iterations, which can be used to calculate a worst case bound for the number of iterations \( k(\epsilon, \rho) \) needed to achieve an accuracy \( \epsilon \). \( x^* \) is the true solution, \( x^k \) the approximate inverse, and \( r^k = D_u x^k - b \) is the residual.

(i) For SUMR we have

\[ \| x^k - x^* \|_2 \leq \frac{1}{\rho - 1} \| r^0_u \|_2 \leq \frac{2}{\rho - 1} \left( \frac{1}{\rho} \right)^k \| r^0 \|_2, \]

\[ k(\epsilon, \rho) \leq \frac{-\ln(\epsilon)}{\ln(\rho)} + \frac{-\ln(2/(\rho - 1))}{\ln(\rho)}. \]

(ii) For MINRES we use \( \| r^0 \|_2 = \| r^0_u \|_2 \), since
\[ r_0^h = \gamma_5 r_0^u, \]
\[ \| x^k - x^* \|_2 \leq \frac{1}{\rho-1} \| r^k \|_2 \leq \frac{2}{\rho-1} \left( \frac{1}{\rho} \right)^{\frac{1}{2}} \| r_0^0 \|_2, \]
\[ \Rightarrow k(\varepsilon, \rho) \leq 2 \left( -\ln(\varepsilon) \frac{1}{\ln(\rho)} + -\ln(2/(\rho-1)) \frac{1}{\ln(\rho)} \right). \]

(iii) For CG (eqn. 3), with two calls to \( D_h \) per iteration) we have
\[ \| x^k - x^* \|_2 \leq 2 \left( \frac{1}{\rho} \right)^k \| x^0 - x^* \|_2 \leq \frac{2}{\rho^k(\rho-1)} \| r^0 \|_2, \]
\[ \Rightarrow k(\varepsilon, \rho) \leq -\ln(\varepsilon) \frac{1}{\ln(\rho)} + -\ln(2/(\rho-1)) \frac{1}{\ln(\rho)}. \]

Based on these worst case estimates, SUMR is a factor 2 faster than CG or MINRES for a propagator calculation. We see this factor of 2 improvement numerically (see figure 1).

3. RELAXATION

While solving \( D_u x = b \), there is no need to calculate the sign function to the full accuracy (\( \equiv \varepsilon \)) during the entire inversion. For each step of the inversion we have to calculate an approximation \( s^j \) to the product of the overlap operator with a vector \( y^j \). Here \( \eta^j \) is the relative accuracy of the sign function:
\[ \| D_u y^j - s^j \| \leq \eta_j \cdot \| D_u \| \cdot \| y^j \|. \]

The precision \( \eta \) can be fixed at a value less than \( \varepsilon \), but it is more efficient to increase \( \eta \) as the inversion progresses. The key is to ensure that the residual gap
\[ \| b - A x^k \| \leq \| r^k - (b - A x^k) \| \text{ true residual} + \| r^k \| \text{ residual gap} + \| r^k \| \text{ computed residual} \]

at the end of the calculation is of order \( \varepsilon \). The optimal relaxation strategies are [1]:

| method   | tolerance \( \eta_j \) |
|----------|------------------------|
| CG       | \( \eta_j = \varepsilon \sqrt{\sum_{i=0}^j \| r^i \|^2} \) |
| MINRES   | \( \eta_j = \varepsilon / \| r^j \| \) |
| SUMR     | \( \eta_j = \varepsilon / \| r^j \| \) |

The accuracy of the sign function can be relaxed by reducing the accuracy of the multishift solver used to solve the ZPFE, and by reducing \( N_Z \). This relaxation can be applied to CG (we call the relaxed CG inversion “relCG”) and SUMR (“relSUMR”). Relaxation gains a factor of 1.5-1.8 in computer time (see section 4).

4. JVE PRECONDITIONING

We can achieve further gains by using inversion of a low-accuracy overlap operator as a preconditioner; we use relSUMR (as preconditioner for the propagator inversion) or relCG (for the full inversion) with the relative accuracy \( \varepsilon = 0.01 \), and \( N_Z = 5 \) (these numbers can be optimized). This preconditioner can be used in an inversion algorithm which can support a variable preconditioner: we used the GMRESR algorithm [5,6]. The GMRESR inversion can be relaxed, using the methods of the previous section, so we have chosen to call this inversion algorithm relGMRESR(SUMR) for the propagator inversion or relGMRESR(CG) for the full inversion. This
preconditioning achieves a gain of at least a factor of 4 in computer time (see figure 2 and tables 1 and 2).

5. CONCLUSIONS

We present algorithms which accelerate the inversion of the overlap operator by a factor of about four for the full inversion (eqn. 3). Using relGMRESR(SUMR) can give a gain of a factor of at least 10 over MINRES for the propagator calculation. We expect that the gain will be increased on larger systems and at lower masses.

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