Deflated BiCGStab for linear equations in QCD problems

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I. Introduction:
The large systems of complex linear equations that are generated in Lattice QCD problems often have multiple right-hand sides (for multiple sources). Deflated GMRES methods[1] have previously been developed for solving multiple right-hand sides. Eigenvectors are generated during solution of the first right-hand side and used to speed up convergence for the other right-hand sides. Here we discuss defating non-restated methods such as BiCGStab[2]. For effective deflation, both left and right eigenvectors are needed. Fortunately, with the Wilson matrix, left eigenvectors can be easily computed. We demonstrate for difficult problems with kappa near kappa critical that defating eigenvalues can significantly improve BiCGStab.

II. Method:
- Consider that a system \( A \xi = \eta \) with \( i = 1,2, \ldots, N \).
- Solve the first system with GMRES-DR(\( m,k \)) with Krylove subspace of dimension \( m \) and deflated right eigenvectors.
- Let \( \Psi_0 \) be an orthonormal basis for the \( k \) right eigenvectors of \( A \) generated during the solution of the first system.
- The left eigenvector basis are given by \( \Psi_0^T \phi \). This relation holds if \( A \) is the Wilson matrix with or without even-odd preconditioning.
- For \( i > 1 \),
  - Let \( \Psi_i \) be the initial guess and \( r_i = b - A x_i \) the initial residual
  - Solve the \( k \times k \) system \( U_i V_i = d \) where
    \[ U_i = \Psi_0^T [A_i - \mu \Psi_0 \Psi_i], \quad V_i = \Psi_i \Psi_0 \]
  - Construct an improved initial guess \( x_{improv} = \Psi_0 y + V d \)
  - Solve the \( \Psi \) system with BiCGStab using \( x_{improv} \) as initial guess.

III. Results for deflated BiCGStab:
- We use a sample of three quenched gauge configurations with Wilson plaquette action at \( \kappa \)-2.0 for the two lattice sizes 16x16 and 20x20.
- The method is applied to the case of Wilson fermions with even-odd preconditioning and kappa critical at maximum twist.
- The first right-hand side is solved with GMRES-DR(\( m,k \)) with residual at convergence \( 1.0 \times 10^{-6} \).
- The accuracy of the eigenvectors generated while solving the first right-hand side increases from \( L_1 \) to \( L_3 \).
- The second right-hand side is solved with BiCGStab and Deflated BiCGStab (D-BiCGStab) using the \( k \) eigenvalues with different accuracy levels \( L_1 \), \( L_2 \), and \( L_3 \).

<table>
<thead>
<tr>
<th>Config. Num.</th>
<th>kappa</th>
<th>GMRES(20) BiCGStab</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.157290</td>
<td>1000 3322</td>
</tr>
<tr>
<td>2</td>
<td>1.157044</td>
<td>1000 3322</td>
</tr>
<tr>
<td>3</td>
<td>1.156810</td>
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Table 1: Number of matrix-vector products for GMRES(20) and BiCGStab for the first r.h.s. on the 20x20 lattice. Residual = 1.0e-08 at convergence and "F" indicates that the method failed to converge.

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<td>1</td>
<td>2.000000</td>
<td>1000 3322</td>
</tr>
<tr>
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<tr>
<td>3</td>
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Table 2: Number of matrix-vector products needed to reach residual 1.0e-08 on the 20x20 lattice for the first-right-hand side (GMRES-DR) and for the second right-hand side (BiCGStab and D-BiCGStab).

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<tr>
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<tr>
<td>3</td>
<td>0.152764</td>
<td>1000 720</td>
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Table 3: Same as in Table 1 for the 16x16 lattice.

IV. A note on multi-mass solvers for Twisted-Mass QCD:
- In Twisted Mass QCD, quarks are introduced as pairs with a modified mass term \( \gamma \mu \gamma \tau \).
- The relation holds for \( \sum_{i=0}^{3} \mu \gamma \tau \) for the 203x32 lattice configurations 1 and 2.
- Solve the first system with GMRES-DR(\( m,k \)) with Krylove subspace of dimension \( k \) and deflated right eigenvectors.
- For \( i > 1 \),
  - Set \( X_0(i) = 0 \) and calculate \( r_0(i) = M(i) X_0(i) - b \)
  - Solve the \( (i-1) \times (i-1) \) system \( [M(i) V]+[M(i) V] y = [M(i) V]+ r_0 \) for \( y \)
  - Solve the system using the improved initial guess with GMRES-DR.
- For \( i > 2 \), use initial guess \( X_0(i) = 0 \) and solve the system using GMRES-DR.
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Table 4: Same as in Table 2 for the 16x16 lattice.

V. Results for the serial multi-mass method:
The method was tested on 20x20 lattice with quenched configurations at \( \kappa = 0 \) with the Wilson plaquette action. The deflated mass fermion action for a degenerate doublet of quarks at maximal twist for 10 values of \( \mu \) is used. The values of \( \mu \) at maximal twist for each value of \( \mu \) are determined using a linear fit of the four \( \langle \Phi_{\mu \mu} \rangle_{\mu \mu} \) values in [8] improvement by a factor of 20-50% was found using the projection step. The efficiency of the method increases as the number of masses to be solved increases and as the separation between successive masses decreases.

VI. Conclusions:
- For problems with multiple right-hand sides with Wilson fermions, a combination of GMRES-DR for the first right-hand side and a deflated BiCGStab for subsequent right-hand sides was tested on typical lattice volumes. It was found to give a considerable reduction of the matrix-vector products by a factor of approximately 5 for the \( L_3 \) case.
- The improvement level increases as the accuracy of the eigenvectors increase.
- Deflated BiCGStab was tested as left-right projection. The methods doesn't add extra work for the case of Wilson fermions where the left eigenvectors are related to the right eigenvectors through \( \Psi \) multiplication.
- For multi-mass problems with multiple masses and even-odd preconditioning, it was found that improving the initial guess using minimal residual projection over previous mass solutions reduces the matrix-vector products by a factor of 20-50%.

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REFERENCES