The two-grid algorithm confronts a shifted unitary orthogonal method

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In this paper I describe a new optimal Krylov subspace solver for shifted unitary matrices called the Shifted Unitary Orthogonal Method (SUOM). This algorithm is used as a benchmark against any improvement like the two-grid algorithm. I use the latter to show that the overlap operator can be inverted by successive inversions of the truncated overlap operator. This strategy results in large gains compared to SUOM.

1. SUOM: A NEW OPTIMAL KRYLOV SOLVER

Consider the task of solving the linear system:

\[ D x = b, \quad D = c_1 1 + c_2 V \]  \hspace{1cm} (1.1)

where \( V = \gamma_5 \text{sign}(H_W) \) is a unitary matrix, \( 1 \) the identity matrix, \( H_W \) the Hermitian Wilson operator, \( c_1 = (1 + m_q)/2, c_2 = (1 - m_q)/2 \) and \( m_q \) the bare fermion mass. The overlap operator \( D \) is non-Hermitian. For such operators GMRES (Generalised Minimal Residual) and FOM (Full Orthogonalisation Method) are known to be the fastest. It is shown that when the norm-minimising process of GMRES converges rapidly, the residual norms in the corresponding Galerkin process of FOM exhibit similar behaviour [3]. But they are based on long recurrences and thus require to store a large number of vectors of the size of matrix columns. However, exploiting the fact that the overlap operator is a shifted unitary matrix one can construct a GMRES type algorithm with short recurrences [4].

Similarly, a short recurrences algorithm can be obtained from FOM. The method is based on an observation of Rutishauser [5] that for upper Hessenberg unitary matrices one can write \( H = LU^{-1} \), where \( L \) and \( U \) are lower and upper bidiagonal matrices. Applying this decomposition for the Arnoldi iteration:

\[ V Q_k = Q_k H_k + h_{k+1,k} q_{k+1} e_k^T \]  \hspace{1cm} (1.2)

one obtains an algorithm which constructs Arnoldi vectors \( Q_k \) by short recurrences [6]:

\[ V Q_k U_k = Q_k L_k + l_{k+1,k} q_{k+1} e_k^T. \]  \hspace{1cm} (1.3)

Projecting the linear system (1.1) onto the Krylov subspace one gets:

\[ (c_1 1 + c_2 L_k U_k^{-1}) y_k = e_1 \]  \hspace{1cm} (1.4)

which can be equivalently written as:

\[ (c_1 U_k + c_2 L_k) z_k = e_1, \quad y_k = U_k z_k. \]  \hspace{1cm} (1.5)

Note that the matrix on the left hand side is tridiagonal. It can be shown that one can solve
this system and therefore the original system using short recurrences [6]. The resulting algorithm is called the Shifted Unitary Orthogonal Method (SUOM) and is given below:

**Algorithm 1 SUOM algorithm**

\[ \rho = ||b||_2; \quad q_0 = b/\rho; \quad w_0 = q_0 \]
\[ l_{00} = q_0^H V q_0 \]
\[ \tilde{q} = V q_0 - l_{00} q_0 \]
\[ l_{10} = ||\tilde{q}||_2; \quad q_1 = \tilde{q}/l_{10} \]
\[ A_{k+1} = ||q||_2 \]
\[ q_{k+1} = q_{k+1}^l \]
\[ l_{kk} = c_1 + c_2 l_{k-1} - c_2 l_{k-1} - l_{k-1} w_{k-1} \]
\[ \alpha_k = c_2 l_{k-1} - l_{k-1} \]
\[ w_k = q_k + u_{k-1} g_k \]
\[ x_k = x_{k-1} + \alpha_k w_k \]
\[ r_k = r_{k-1} - \alpha_k D w_k \]
\[ \text{Stop if } ||r_k||_2 < \text{tol} \rho \]

Note that in an actual implementation one can store \( V q \) and \( D w \) as separate vectors, which can be used in the subsequent iteration to compute \( D w_{k+1} \). Therefore only one multiplication by \( V \) is needed at each step.

2. THE TWO-GRID ALGORITHM

A straightforward application of multigrid algorithms is hopeless in the presence of non-smooth gauge fields. However, the situation is different for the 5-dimensional formulation of chiral fermions where there are no gauge connections along the fifth dimension. Here, I will limit my discussion in the easiest case which consists of two grids: the “fine” grid, which is the continuum along the fifth coordinate and a coarse grid, which is the lattice discretisation of the “fine” grid.

I define chiral fermions on the coarse grid using truncated overlap fermions [7]. The corresponding 5-dimensional matrix \( \mathcal{M} \) in blocked form is given by:

\[
\begin{pmatrix}
D_W - I & (D_W + I)P_+ & -m_q(D_W + I)P_- \\
(D_W + I)P_- & \ddots & \ddots \\
-m_q(D_W + I)P_+ & \ddots & \ddots & \ddots
\end{pmatrix}
\]

where \( P \pm = (I \pm \gamma_5)/2 \). Let \( \mathcal{M}_1 \) be the above matrix but with bare quark mass \( m_q = 1 \) and \( P \) the permutation matrix:

\[
\begin{pmatrix}
P_+ & P_- \\
P_+ & \ddots \\
& \ddots & P_-
\end{pmatrix}
\]

It can be shown that the following result hold [2,8]:

**Proposition 2.1** Let \( P^T \mathcal{M}_1^{-1} \mathcal{M}P \chi = \eta \) be the linear system defined on the 5-dimensional lattice with \( \chi = (y, \chi^{(2)}, \ldots, \chi^{(N)})^T \) and \( \eta = (r, o, \ldots, o)^T \). Then \( y \) is the solution of the linear system \( D^{(N)} y = r \), where \( D^{(N)} \to D \) as \( N \to \infty \).

This result lends itself to a special two-grid algorithm [2,8]. Indeed, \( x_5 = a_5 \) is the (fifth Euclidean) coordinate of interest since it contains the information about the 4-dimensional physics. One way of exploiting this is to use “decimation”

**Algorithm 2 The two-grid algorithm**

\[ x_5 \in \mathbb{C}^N; \quad r_5 = b - D x_5; \quad \text{tol}, \text{tol}_0 \in \mathbb{R}_+ \]

for \( i = 1, 2, \ldots \) do

Let \( \eta_i = (r_1, o, \ldots, o)^T \in \mathbb{C}^{N_5} \)

Let \( \chi_{i+1} = (y_{i+1}, \chi_{i+1}^{(2)}, \ldots, \chi_{i+1}^{(N)})^T \in \mathbb{C}^{N_5} \)

Solve \( \mathcal{M}_1 \mathcal{P}_{\chi_{i+1}} = \mathcal{M}_1 \mathcal{P}_{\eta_i} \) until

\[ ||\mathcal{M}_1 P_{\eta_i} - \mathcal{M}_1 P_{\chi_{i+1}}||_2 < \text{tol}_0 \]

\[ x_{i+1} = x_i + y_{i+1} \]

\[ r_{i+1} = b - D x_{i+1} \]

Stop if \( ||r_{i+1}||_2 < \text{tol} \)

end for

over the fifth coordinate in order to get the 5d-vector \( \eta \). Using proposition 2.1 one can evaluate directly the first 4d-component of \( \eta \) by \( r = b - D x \), \( x \) being an approximate solution. The rest can be
padded with zero 4d-vectors. The second step is to solve the problem on the coarse grid. Finally, one can extract the 4d-solution \( y \) on this grid and correct the “fine” grid solution by \( x \leftarrow x + y \). In the second cycle one has to repeat the same decimation method, since the “fine” 5d-operator is not available. Hence, the whole scheme is a restarted two-grid algorithm, which is given here as Algorithm 2.

3. COMPARISON OF METHODS

In Fig. 1 is shown the convergence of various algorithms as a function of Wilson matrix-vector multiplication number on a fixed gauge background on a \( 8^316 \) lattice at \( \beta = 5.7 \). The convergence is measured using the norm of the residual error. For the overlap matrix-vector multiplication is used the double pass Lanczos algorithm (without small eigenspace projection of \( H_W \)) as described in [9]. Together with the algorithms described in the previous sections Fig. 1 shows the performance of Conjugate Residuals (CR), Conjugate Gradients on Normal Equations (CGNE) and CG-CHI. The latter is the CGNE which solves simultaneously the decoupled chiral systems appearing in the matrix \( D^H D \). One can observe a gain over CGNE which may be explained due to the reduced number of eigenvalues at each chiral sector. However, this gain is no more than 10%. On the other hand SUOM and CR perform rather similar with SUOM being slightly faster in this scale. The gain over CGNE is about a factor two. The Two-Grid algorithm performs the best with a gain of at least a factor 6 over SUOM and more than an order of magnitude over CGNE. This situation repeats itself for a different gauge configuration which is not shown here for the lack of space. However, if the projection of small eigenvalues is used the gain over SUOM/CR should be smaller since the Two-Grid algorithm is much less intensive in the application of the overlap operator. It is exactly the purpose of this comparison to make clear this feature of the Two-Grid algorithm. Finally, it is (not) surprising that SUOM and CR perform similarly: CR can be shown to be an efficient method for normal matrices. Since it is easier to imple-

![Figure 1. Norm of the residual as a function of the number of \( D_W(M) \) multiplications for different algorithms for \( M = -1.8 \)](image)

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