Many masses on one Stroke: Economic Computation of Quark Propagators

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October 20, 2018

Abstract

The computational effort in the calculation of Wilson fermion quark propagators in Lattice Quantum Chromodynamics can be considerably reduced by exploiting the Wilson fermion matrix structure in inversion algorithms based on the non-symmetric Lanczos process. We consider two such methods: QMR (quasi minimal residual) and BCG (biconjugate gradients).

Based on the decomposition \( M/\kappa = 1/\kappa - D \) of the Wilson mass matrix, using QMR, one can carry out inversions on a whole trajectory of masses simultaneously, merely at the computational expense of a single propagator computation. In other words, one has to compute the propagator corresponding to the lightest mass only, while all the heavier masses are given for free, at the price of extra storage.

Moreover, the symmetry \( \gamma_5 M = M^T \gamma_5 \) can be used to cut the computational effort in QMR and BCG by a factor of two. We show that both methods then become—in the critical regime of small quark masses—competitive to BiCGStab and significantly better than the standard MR method, with optimal relaxation factor, and CG as applied to the normal equations.
1 Introduction

Lattice QCD allows to compute physical quantities like the hadronic spectrum, weak decay constants and other weak matrix elements without recourse to perturbation theory [1]. Basic building blocks for the construction of such observables are the quark propagators, i.e. the Green’s functions of the fermionic operator. In practice, the latter are determined via an iterative inversion method on an ensemble of gauge background fields, generated in a Monte Carlo process. Thus, the evaluation of quark propagators represents a major task within this branch of elementary particle theory.

One can work in two directions in order to achieve good efficiency computing the propagators:

- acceleration of the convergence using improved iterative procedures [2, 3],
- exploitation of the structure of the matrix $M$ in the implementation of the inverter.

Of course, these two directions are not mutually exclusive.

In this note we go one step into the second direction and point out how the structure of $M$ can be exploited in iterative methods based on the non-symmetric Lanczos process [4]. Specific methods in this class comprise the BCG (biconjugate gradient) method of Fletcher [5] and the more recent QMR (quasi minimum residual) method of Freund and Nachtigal [6]. We show that these Lanczos based methods can be very useful in carrying out the extrapolation to the chiral limit: one can perform inversions on a whole trajectory of masses simultaneously. In other words, one has to compute the propagator corresponding to the lightest mass only, while all the heavier masses are almost given for free, at the price of extra storage.

Moreover, we shall also point out how the particular symmetry properties of the Wilson fermion matrix can be used to further reduce the costs of each iterative step in QMR or BCG by a factor of 2. This fact, mentioned in Ref. [7] has recently attracted attention in the lattice QCD community.

After discussing the basic properties of the Wilson fermion matrix in Section 2, we will present the QMR and BCG algorithms in quite some detail (Section 3) and explain the savings in computational effort due to the structure of the Wilson fermion matrix. Section 4 contains the results of our numerical experiments on the CM5 parallel computer at Wuppertal university. In particular, we will compare the QMR algorithm with BiCGStab
BCG and with the standard over-relaxed MR (minimal residuum) method [8] on realistic configurations for different values of $\kappa$, approaching the critical regime of very small relative quark masses. All these calculations were done using standard odd-even preconditioning.

2 Basic properties of the Wilson fermion matrix

The Dirac operator in its discretized form as given by Wilson [10] reads:

$$M = 1 - \kappa D,$$

(1)

with the off-diagonal hopping term

$$D_{x,y} = \sum_{\mu=1}^{4} \left( (1 - \gamma_{\mu}) U_{\mu}(x) \delta_{x,y-\mu} + (1 + \gamma_{\mu}) U_{\mu}^{\dagger}(x-\mu) \delta_{x,y+\mu} \right).$$

(2)

In Eq. 2, the $\{U_{\mu}(x)\}$ represent the gauge background field on a four-dimensional Euclidean space-time lattice.

In the following it is preferable to scale $M$ by a factor $\frac{1}{\kappa}$: $M \rightarrow \frac{1}{\kappa} M$. We shall thus consider the solution of the linear equation

$$Mx = (\frac{1}{\kappa} 1 - D)x = \phi.$$  

(3)

The matrix $M = \frac{1}{\kappa} 1 - D$ in Eq. 3 has two important properties which will be crucial to algorithms for solving Eq. 3:

• $M$ is $\gamma_5$-symmetric, i.e.

$$M \gamma_5 = \gamma_5 M^\dagger$$

where $\gamma_5$ is the permutation matrix which commutes the Dirac components 1 with 3 and 2 with 4 on each lattice site. In particular, $\gamma_5$ is unitary and hermitian:

$$\gamma_5 = \gamma_5^\dagger = \gamma_5^{-1}.$$  

Multiplying a vector by $\gamma_5$ is a very cheap operation.

• $M$ is a shifted matrix with respect to its dependence on $\kappa$, i.e. $M$ is the sum of a multiple of the identity and a constant off-diagonal part $D$. 

3
When building up $M$ one has the freedom to choose any ordering scheme for the lattice sites. Subdividing the lattice in a checkerboard style into even and odd sites and numbering all even sites before the odd ones results in the following two-cyclic structure for $M$

\[
M = \begin{pmatrix}
\frac{1}{\kappa}1 & -D_{eo} \\
-D_{oe} & (1/\kappa)1
\end{pmatrix}.
\]

(4)

Using the indices ‘e’ and ‘o’ to denote even and odd sites, respectively, we can thus rewrite Eq. 3 as

\[
\begin{pmatrix}
\frac{1}{\kappa}1 & -D_{eo} \\
-D_{oe} & (1/\kappa)1
\end{pmatrix}
\begin{pmatrix}
x_e \\
x_o
\end{pmatrix}
= \begin{pmatrix}
\phi_e \\
\phi_o
\end{pmatrix}
\]

This equation separates into

\[
M_e x_e = \tilde{\phi}_e,
\]

(5)

\[
x_o = \kappa \cdot (\phi_o + D_{oe} x_e),
\]

(6)

where

\[
M_e = \frac{1}{\kappa^2}1 - D_{eo} D_{oe},
\]

(7)

\[
\tilde{\phi}_e = \frac{1}{\kappa} \phi_e + D_{oe} \phi_0.
\]

(8)

Eq. 5 is called the odd-even preconditioned system [11, 12], with $M_e$ given by Eq. 7. It has become standard to solve the odd-even preconditioned system rather than the original one since iterative methods for Eq. 3 converge faster than for Eq. 3.

In our context, it is very important to notice that the matrix $M_e$ of the preconditioned system conserves both basic properties of $M$ as stated before, i.e. $M_e$ is still $\gamma_5$-symmetric and a shifted matrix (with factor $1/\kappa^2$ instead of $1/\kappa$). Therefore, using QMR or BCG we can take advantage of the particular structure of $M_e$ in just the same manner as with $M$. However, one should be aware of that the new source term $\tilde{\phi}_e$ in Eq. 8 will depend on $\kappa$ as soon as $\phi_e \neq 0$. This must be accounted for when exploiting the shifted structure of $M_e$. Details will be given in the next section.
3 QMR and BCG

We consider two different iterative methods for solving Eq. 3: The BCG (biconjugate gradient) method of Fletcher [5] and the QMR (quasi minimum residual) method of Freund and Nachtigal [6]. Generic formulations for these methods are given in Algorithms 1 and 2, see also Ref. [13]. Although QMR looks somewhat more involved than BCG, both methods require approximately the same computational work per iteration: One matrix multiplication with $M$ and another with $M^\dagger$, the additional scalar and vector operations being negligible in either method. QMR will usually reduce the norm of the residual in a much smoother manner than BCG does, thus making QMR more stable numerically.

choose $x^0 \in \mathbb{C}^n$, set $p^0 = r^0 = \phi - Mx^0$

choose $\tilde{r}^0 \in \mathbb{C}^n$, set $\tilde{p}^0 = \tilde{r}^0$

for $m = 0, 1, \ldots$

$\delta_m = (\tilde{r}^m)^\dagger r^m / (\tilde{p}^m)^\dagger Mp^m$

$x^{m+1} = x^m + \delta_m p^m$

$r^{m+1} = r^m - \delta_m Mp^m$

$\tilde{r}^{m+1} = \tilde{r}^m - \delta_m M^\dagger \tilde{p}^m$

$\rho_m = (\tilde{r}^{m+1})^\dagger r^{m+1} / (\tilde{r}^m)^\dagger r^m$

$p^{m+1} = p^{m+1} + \rho_m p^m$

$\tilde{p}^{m+1} = \tilde{r}^{m+1} + \rho_m \tilde{p}^m$

Algorithm 1: BCG method.

The vectors $\tilde{r}^0$ in BCG and $\bar{w}^0$ in QMR can be chosen freely. If we take $\tilde{r}^0 = \bar{w}^0$, it can be shown [14] that $r^m_{BCG}$ is a scalar multiple of $\bar{v}^m$ and $\tilde{r}^m$ is a scalar multiple of $\bar{w}^m$. (We use the subscripts BCG and QMR to distinguish between quantities which are otherwise denoted by the same symbol in both methods). Thus, QMR and BCG are intimately related and one can show that [14]

$$x^m_{BCG} = x^m_{QMR} - \mu_m s_m p_{QMR}^m$$

and

$$\|r^m_{BCG}\| = \|r^0\|_2 \cdot |s_1 \ldots s_m| \cdot \frac{1}{c_m}.$$
choose $x^0 \in \mathbb{C}^n$, set $\tilde{v}^0 = b - Mx^0$
choose $\tilde{w}^0 \in \mathbb{C}^n$

{initialize}
set $\mu_0 = \|\tilde{v}^0\|$, $\delta_0 = 1$, $c_{-1} = c_0 = 1$, $s_{-1} = s_0 = 0$ ,
set $p^{-1} = p^{-2} = v^{-1} = w^{-1} = 0$
for $m = 0, 1, \ldots$

{next Lanczos step}
\begin{align*}
\rho_m &= \|\tilde{v}^m\|, \quad \eta_m = \|\tilde{w}^m\| \\
\tilde{v}^m &= \tilde{v}^m / \rho_m, \quad \tilde{w}^m = \|\tilde{w}^m\|\eta_m \\
\delta_m &= (\tilde{w}^m)^\dagger v^m \\
\alpha_m &= (\tilde{w}^m)^\dagger M\tilde{v}^m / \delta_m \\
\beta_m &= \eta_m \delta_m / \delta_{m-1}, \quad \gamma_m = \rho_m \delta_m / \delta_{m-1} \\
\tilde{v}^{m+1} &= M\tilde{v}^m - \alpha_m \tilde{v}^m - \beta_m \tilde{v}^{m-1} \\
\tilde{w}^{m+1} &= M^\dagger \tilde{w}^m - \alpha_m \tilde{w}^m - \gamma_m \tilde{w}^{m-1}
\end{align*}

{update QMR recurrence coefficients}
set $\Theta_{m+1} = s_{-m-1} \beta_m, \tilde{\varepsilon}_{m+1} = c_{-m-1} \beta_m, \varepsilon_{m+1} = c_m \tilde{\varepsilon}_{m+1} + s_m \alpha_m, \tilde{\delta}_{m+1} = -s_m \tilde{\varepsilon}_{m+1} + c_{m} \alpha_m, \nu_{m+1} = (|\tilde{\delta}_{m+1}|^2 + |\gamma_{m+1}|^2)^{1/2}, c_{m+1} = |\tilde{\delta}_{m+1}| / \nu_{m+1}, \tilde{\tau}_{m+1} = 0$ if $\tilde{\delta}_{m+1} = 0, \tilde{\tau}_{m+1} = c_{m+1} \gamma_{m+1} / \tilde{\delta}_{m+1}$ if $\tilde{\delta}_{m+1} \neq 0, \delta_{m+1} = c_{m+1} \tilde{\delta}_{m+1} + s_{m+1} \gamma_{m+1}$
{update QMR iterate}
set $p^m = (\tilde{v}^m - \varepsilon_{m+1} p^{m-1} - \Theta_{m+1} p^{m-2}) / \delta_{m+1}$
\begin{align*}
\bar{\mu}_m &= c_{m+1} \mu_m \\
x^{m+1} &= x^m + \bar{\mu}_m p^m \\
\mu_{m+1} &= \tilde{\tau}_{m+1} \mu_m
\end{align*}

Algorithm 2: QMR method.
So, the BCG iterates can be retrieved very easily from the QMR iterates. The generation of $v^m$ and $w^m$ as given in the QMR algorithm is called the non-symmetric Lanczos process. This process is the common basis of QMR and BCG.

Both methods, QMR and BCG can break down prematurely due to $\delta_m = 0$ in QMR or zero divisors in $\rho_m$ or $\delta_m$ in BCG. This is why the state-of-the-art package QMRPACK [15] (distributed freely through the netlib server netlib@ornl.gov) contains modifications of QMR in which ‘look-ahead’ Lanczos steps [16] are incorporated. This avoids premature breakdowns at the expense of extra storage and it further enhances the numerical stability.

choose $x^0 \in \mathbb{C}^n$, set $p^0 = r^0 = \phi - Mx^0$

for $m = 0, 1, \ldots$

$\delta_m = (\gamma_5 r^m)^\dagger r^m / (Ap^m)^\dagger (\gamma_5 p^m)$

$x^{m+1} = x^m + \delta_m p^m$

$r^{m+1} = r^m - \delta_p A p^m$

$\rho_m = (\gamma_5 r^{m+1})^\dagger r^{m+1} / (\gamma_5 r^m)^\dagger r^m$

$p^{m+1} = r^{m+1} + \rho_m p^m$

Algorithm 3: BCG exploiting the $\gamma_5$-symmetry.

If we choose $\tilde{r}^0 = \gamma_5 r^0$ in BCG, an easy calculation shows that due to the $\gamma_5$-symmetry of $M$ we have $\tilde{r}^m = \gamma_5 r^m$ for all $m$ and the scalars $\delta_m, \rho_m$ in BCG are all real. Consequently, the computational effort per iteration reduces to only one matrix multiplication, see Algorithm 4. Similarly, if we take $\tilde{v}^0 = \gamma_5 v^0$ in QMR, the non-symmetric Lanczos step yields $\tilde{w}^m = \gamma_5 \tilde{v}^m$ for all $m$ and the scalar quantities in QMR again become all real. This simplified version of the Lanczos process is given in Algorithm 4. So, once more, the multiplication with $M^\dagger$ can be saved, reducing the computational effort in QMR by a factor of two. In the more general case of so-called $P$-symmetric matrices, the above simplifications were already described in Ref. [17].

Additionally, we note that $M$ being a shifted matrix, $M = \sigma I - D$ with $\sigma = 1/\kappa$, we can rewrite the generation of $\tilde{v}_m$ in the non-symmetric Lanczos process of Algorithm 4 as

$$
\tilde{v}^m = -Dv^{m-1} - (\alpha_{m-1} - \sigma)v^{m-1} - \beta_{m-1}v^{m-2},
$$
choose \( \overline{v}^0 \)
set \( v^{-1} = 0, \quad \delta_0 = 1 \)
for \( m = 0, 1, \ldots \)
\[
\rho_m = \|\overline{v}^m\| \\
v^m = \overline{v}^m / \rho_m \\
\delta_m = (\gamma_5 v^m)^\dagger v^m \\
\alpha_m = (\gamma_5 v^m)^\dagger M v^m / \delta_m \\
\beta_m = \rho_m \delta_m / \delta_m - 1 \\
\overline{v}^{m+1} = M v^m - \alpha_m v^m - \beta_m v^{m-1}
\]

Algorithm 4: The non-symmetric Lanczos process exploiting \( \gamma_5 \)-symmetry.

with
\[
\alpha_{m-1} - \sigma = (\gamma_5 v^{m-1})^\dagger (-D) v^{m-1} / \delta_{m-1}.
\]
This shows that the Lanczos vectors \( \overline{v}^m \) and \( v^m \) depend only on \( D \) but not on \( \sigma \), provided one always has the same initial vector \( \overline{v}^0 \). The recurrence coefficients \( \beta_m, \eta_m \) remain unchanged whereas the coefficient \( \alpha_m \) changes to \( \alpha_m + \sigma \) if we change the matrix from \( -D \) to \( \sigma 1 - D \).

Consequently, if we simultaneously solve several systems
\[
\left( \frac{1}{\kappa_i} 1 - D \right) x_i = \phi, \quad i = 1, \ldots, l
\]
using QMR, the Lanczos part itself has to be performed only once, provided we take the initial guess \( x^0_i = 0 \) for \( i = 1, \ldots, l \). In fact, \( x^0_i = 0 \) for \( i = 1, \ldots, l \) leads to the same initial residual \( r^0_i = \phi \) for \( i = 1, \ldots, l \) so that \( \overline{v}^0 = \phi \) represents the initial vector of the Lanczos process for all \( i \). These observations go back to Ref. [18].

Note that the odd-even preconditioned system Eq. [3] has the same shifted structure as the original Wilson-Fermion matrix with \( \sigma = 1/\kappa^2 \). The right hand side \( \overline{\phi}_e = \frac{1}{\kappa} \phi_e + D_{oe} \phi_0 \), however, will usually depend on \( \kappa \) so that it is impossible to easily find initial guesses which lead to the same initial residual. In that case we propose to consider the two systems
\[
M_e y_e = \phi_e \\
M_e z_e = D_{oe} \phi_0
\]
which now both leave an initial residual that does not depend on \( \kappa \) if the initial guess is taken to be zero. Hence, again, for each of the two systems
the non-symmetric Lanczos process needs to be performed only once for different values of $\kappa$.

So, in the QMR method we can treat several values of $\kappa$ at the same time without introducing any additional matrix multiplications. This also holds for the BCG iterates if we compute them from the QMR algorithm via Eq. 8. The price to pay is 4 vectors extra storage for each additional value of $\kappa$. This can be reduced to 3 vectors if we refrain from updating the residuals. Indeed, it was shown in Ref. [6] that

$$\|r^m\| \leq \|r^0\|_2 \cdot \sqrt{m+1} \cdot |s_1, \ldots, s_m| =: \tau_m .$$

The scalar $\tau_m$ can be updated easily, and since it represents an upper bound for $\|r^m\|$ it can be used in a stopping criterion. It has turned out to be a good choice checking for $\tau_m \leq 10 \cdot \varepsilon$ if one wants to have $\|r^m\| \leq \varepsilon$, but, of course, the latter inequality should be re-checked by explicitly computing $r^m$ and $\|r^m\|$ once $\tau_m \leq 10 \cdot \varepsilon$ is fulfilled.

Finally, we just mention that all the above simplifications remain valid if we incorporate the look-ahead Lanczos process [9].

4 Results

Our numerical computations were done on the CM5 parallel computer at Wuppertal university. We tested and compared five different methods for solving the odd-even preconditioned system Eq. 5: QMR and BCG as described before, the standard over-relaxed MR (minimal residual) method, the BiCGStab method and the usual conjugate gradient method applied to the normal equation

$$M_e^\dagger M_e x_e = M_e^\dagger \tilde{\phi}_e.$$ 

This method is abbreviated CGNE.

In our comparative study, we set high value on trying to be close to realistic lattice gauge applications: at $\beta = 6.0$, we have generated an ensemble of 10 decorrelated quenched gauge configurations on a lattice of size of $16^4$, see also Ref. [8]. We worked with a series of $\kappa$-values, $\kappa = 0.152, 0.153, 0.154, 0.155, 0.1553$, that corresponds to a quark mass range $0.1 > m_q > 0.03$. In Refs. [19, 20, 21], propagator computations on these $\kappa$-values resulted in a nearly linear pion mass trajectory as function of $1/\kappa$.

As is well known that the convergence behaviour of iterative solvers can depend on the source vector, we adapted the Wuppertal source smearing
method [22] to build our source: starting from a location $x$ on a given time-slice the smeared source is generated according to the smearing procedure

$$\phi(x,t) \rightarrow \phi'(x,t) = \frac{1}{1 - 6\alpha} \times \left\{ \phi(x,t) + \alpha \sum_{i=1}^{3} \left[ U_i(x, t) \phi(x + \vec{e}_i, t) + U_i^\dagger(x - \vec{e}_i, t) \phi(x - \vec{e}_i, t) \right] \right\},$$

(12)

with the unit vector $\vec{e}_i$ pointing in spatial direction $i$. We used $\alpha = 4$ and performed 100 smearing iterations.

Our first diagram (Figure 1) reports result obtained on one given configuration of the ensemble with a smeared source and $\kappa = 0.155$. We display the convergence history for the different methods by plotting the norm of the residual (normalized to $\|r^0\| = 1$) against the number of matrix multiplications involved. Since in either method all the computational effort is very highly concentrated on the matrix multiplications, Figure 1 may also be interpreted as giving the norm of the residuals as a function of computing time. Here, a matrix multiplication is a multiplication with $M_e$ or $M_e^\dagger$. Note that each iterative step of CGNE and BiCGStab requires two matrix multiplications, whereas MR, QMR and BCG require only one since we take advantage of the $\gamma_5$-symmetry. In all methods, our starting vector was the zero vector. In BiCGStab, the ‘shadow residual vector’ $\hat{r}^0$ was chosen equal to the initial residual, which means that we used BiCGStab exactly as described in Ref. [3].

Figure 1 shows that CGNE is by far the slowest method and that MR also performs substantially worse than the remaining three methods, although we used the optimal relaxation factor in MR. This factor was found to be 1.1 by numerical experimentation. Figure 1 also illustrates the wide fluctuations in the residual norm which one usually observes in BCG. On the other hand, QMR converges very smoothly. The speed of convergence of all three methods, QMR, BCG and BiCGStab looks quite comparable, with BiCGStab being slightly better at the beginning, whereas BCG and QMR perform a little better towards the end. To reach the required residual norm of $10^{-10}$, QMR and BCG were the fastest of all methods with QMR performing some 10% better than BiCGStab. If we had not made use of the $\gamma_5$-symmetry, both methods would have taken twice the number of matrix multiplications so that both methods would become clearly inferior to BiCGStab. This is the reason why, based on computations on a cold
Figure 1: Convergence history for different methods
and a hot model configuration and without exploiting $\gamma_5$-symmetry QMR and BCG were regarded as less efficient than BiCGStab and its variant BiCGStab2 in Ref. [2].

We now turn to demonstrate the additional savings possible by exploiting the $\gamma_5$-symmetry together with the shifted structure of the Wilson fermion matrix. We compare QMR-MULT, the QMR method for solving Eq. [1] on an entire set of $\kappa$-values simultaneously (so the Lanczos process is carried out only once), with a standard sequential computation on these $\kappa$ values. To make a fair comparison, we used the educated guess technique in the latter case, i.e. the final result of a computation for which the previous $\kappa$ was taken as the new starting vector for the next $\kappa$. For this serial treatment of the different values of $\kappa$ we tried CGNE, over-relaxed MR, BiCGStab and QMR itself. For these comparisons we used the whole ensemble of 10 configurations. The results for CGNE were so inferior in comparison to the other methods that we decided to not include them into our diagrams.

Figure 2 gives the total number of matrix multiplications $m$ as a function of the number of $\kappa$'s for which the calculations have been done. More precisely, a value of $i$ on the horizontal axis refers to the calculation of $i$ different values $\kappa_1, \ldots, \kappa_i$, where

$$\kappa_1 = 0.152, \quad \kappa_2 = 0.153, \quad \kappa_3 = 0.154, \quad \kappa_4 = 0.155, \quad \kappa_5 = 0.1553.$$  

In Figure 2, the source term was taken to be a point source. The initial vector was the zero vector for all $\kappa$'s in QMR-MULT and for the first value of $\kappa$ in all other methods. As a consequence, a look-ahead Lanczos step had to be performed in QMR and QMR-MULT at the very beginning of the iteration due to $(\gamma_5 \phi_e)^\dagger \phi_e = 0$. We used a simple modification of Algorithm 4 to perform this look-ahead step.

In either method the iteration was stopped when the norm of the residual, weighted by the norm of the source term (which is the initial residual if we take starting vector zero) was less than $10^{-10}$. The representation in Figure 2 shows the average values over the whole sample of 10 configurations. The deviation of the results for the individual configurations from the average was quite small, ranging from less than 2% for small values of $\kappa$ to never more than 10% for the largest $\kappa$ in either method.

Figure 3 refers to exactly the same computations as Figure 2, showing now the computing time on the CM5 as a function of the number of $\kappa$'s.

\footnote{A more elaborate implementation of the QMR method exploiting $\gamma_5$-symmetry and the shifted structure based on QMRPACK is currently under development.}
comparison with Figure 2 very clearly establishes that the computing time is proportional to the number of matrix multiplications. Of course, in QMR-MULT, the additional work to be spent in updating the iterates increases as we treat more $\kappa$'s simultaneously, but this only minorly affects the overall computing time.

Figure 2 and 3 show that the more values of $\kappa$ we treat simultaneously in QMR-MULT, the more we gain in computing time against the educated guess variants. While for the case of one single $\kappa$ all methods perform comparably well, the ‘several-on-one-stroke’ approach pays out as soon as we treat 2 or more values of $\kappa$ simultaneously. For 5 values of $\kappa$, QMR-MULT is almost three times as fast as the most rapid educated guess method (via BiCGStab).

As was pointed out at the end of Section 2, using other sources than point sources will usually require QMR-MULT to be performed on two sys-
tem with different source terms, whereas this is not necessary for the other methods. In that case we thus expect the QMR-MULT approach to become approximately two times more slowly. Nevertheless, it would be faster than all methods based on the educated guess as soon as we treat 4 or more values of $\kappa$ simultaneously. For 5 values of $\kappa$, for example, QMR-MULT will still be some 50% better than BiCGStab.

## 5 SUMMARY

In this note we have presented and tested an extension of the QMR algorithm, the QMR-MULT, which exploits structural and symmetry properties of the Wilson Fermion matrix in order to speed up the inversions on a whole
mass trajectory. In the setting of a realistic application, we have shown that the QMR-MULT can save a factor two to four in computer time, compared to the fastest algorithms which are presently in use.

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