SIAM J. SCI. COMPUT.
Vol. 23, No. 2, pp. 363–380

FQMR: A FLEXIBLE QUASI-MINIMAL RESIDUAL METHOD WITH INEXACT PRECONDITIONING*

DANIEL B. SZYLD† AND JUDITH A. VOGEL‡

Abstract. A flexible version of the QMR algorithm is presented which allows for the use of a different preconditioner at each step of the algorithm. In particular, inexact solutions of the preconditioned equations are allowed, as well as the use of an (inner) iterative method as a preconditioner. Several theorems are presented relating the norm of the residual of the new method with the norm of the residual of other methods, including QMR and flexible GMRES (FGMRES). In addition, numerical experiments are presented which illustrate the convergence of flexible QMR (FQMR), and show that in certain cases FQMR can produce approximations with lower residual norms than QMR.

Key words. Krylov subspace methods, flexible preconditioning, inner-outer iterations

AMS subject classification. 65F10

PII. S106482750037336X

1. Introduction.

The quasi-minimal residual (QMR) method [11] is a well-established Krylov subspace method for solving large systems of non-Hermitian linear equations of the form

$$A\mathbf{x} = \mathbf{b}, \tag{1}$$

where the $n \times n$ matrix A is assumed to be nonsingular. The algorithm makes use of a three-term recurrence, and thus, unlike some other Krylov methods for non-Hermitian systems, e.g., GMRES [23], storage requirements are fixed and known a priori.

The strength of Krylov subspace methods is most apparent when a preconditioner is used. For a general introduction to these methods see, e.g., [17], [22]. In the case of right preconditioning, one solves the equivalent linear system

$$AM^{-1}(M\mathbf{x}) = \mathbf{b}$$

with some appropriate preconditioner M. The matrix AM^{-1} is never formed explicitly. Instead, when $\mathbf{z} = M^{-1}\mathbf{v}$ is required, one solves the corresponding system

$$M\mathbf{z} = \mathbf{v}. \tag{2}$$

In an analogous manner, left preconditioning consists of solving $M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$.

In this paper we present a flexible version of QMR, where the matrix M in (2) can vary from one iteration to the next. Let us denote by M_i the preconditioner used at the ith iteration. The need to allow for a variable preconditioner arises, e.g., when the solution of (2) is not obtained exactly (say, by a direct method), but is approximated by the use of a second (inner) iterative method. This is the case, e.g., when the preconditioner used is some version of multigrid, such as in [10].

*Received by the editors June 7, 2000; accepted for publication (in revised form) December 21, 2000; published electronically July 10, 2001.
http://www.siam.org/journals/sisc/23-2/37336.html

†Department of Mathematics, Temple University (038-16), 1805 N. Broad Street, Philadelphia, PA 19122-6094 (szyld@math.temple.edu). The work of this author was supported by the National Science Foundation grant DMS-9973219.

‡Richard Stockton College, Pomona, NJ 08240 (judith.vogel@stockton.edu).

In recent years, several authors worked on the idea of preconditioning with a different matrix at each outer iteration of a Krylov subspace method [1], [16], [20], [21], [25]; see also [6], [14], [15] for other instances of inner-outer iterations. Preconditioning of this form is referred to as flexible preconditioning, also known as variable or inexact preconditioning. Our approach to a flexible version of QMR, which we call FQMR, is similar to that of Saad for FGMRES [21]. In addition, we were influenced by ideas presented by Golub and Ye for inexact conjugate gradients [16].

The new FQMR method, in the same way as the other inexact methods just mentioned, is not strictly speaking a Krylov subspace method. This is because the minimization at each step is done over a subspace which is not in general a Krylov subspace; also cf. [7]. Nevertheless, the convergence theory developed by Eiermann and Ernst [9] applies to these methods as well.

We emphasize that FQMR can be used whenever FGMRES is used, with the advantage that FQMR has a fixed low memory requirement.

FQMR is not intended as an alternative to QMR when the latter works well but rather as an option when no fixed preconditioner is available, as in [10] and in [18], or when the preconditioner can be improved from one step to the next with newly available information; cf. [2]. Nevertheless, we have found in our numerical experiments that FQMR can produce approximations with lower residual norms than QMR.

In the next section we briefly review the QMR method and present the new flexible version. We describe several properties of this new version, including the quasi-minimization property over a certain subspace. In section 3 we present our main theorem relating the residual norm of FQMR with that of FGMRES, in a way analogous to the well-known relation between QMR and GMRES. As a corollary we obtain a new relation between the residual norm of FGMRES and that of QMR.

The same techniques are used in section 4 to obtain bounds for the FQMR residual norm. As is to be expected, these bounds are in terms of how inexactly each preconditioned step is solved. In a similar way new bounds for the FGMRES residual norm are obtained.

Finally, in section 5 numerical experiments are reported which describe the convergence behavior of FQMR using several different iterative methods as flexible preconditioners. Furthermore, a comparison is made between FQMR and the corresponding version of QMR with fixed preconditioner. This comparison shows that in many cases the maximal attainable accuracy of FQMR, i.e., the minimum relative residual norm, is better than that of QMR.

2. The FQMR algorithm.

We begin this section by first considering the standard QMR algorithm with a fixed right preconditioner M; for full details see [11], [17], or [22]. An analogous description can be given for QMR with fixed left preconditioning. Let $\mathbf{x}_0$ be the initial guess and let $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$ be the initial residual. In QMR, the two-sided Lanczos algorithm is used to construct biorthogonal bases corresponding to the Krylov subspaces generated by AM^{-1} and $(AM^{-1})^H$, namely,

$$K_m(AM^{-1}, \mathbf{r}_0) = \operatorname{span}\{\mathbf{r}_0, AM^{-1}\mathbf{r}_0, \ldots, (AM^{-1})^{m-1}\mathbf{r}_0\}$$

and

$$K_m((AM^{-1})^H, \mathbf{r}_0) = \operatorname{span}\{\mathbf{r}_0, M^{-H}A^H\mathbf{r}_0, \ldots, (M^{-H}A^H)^{m-1}\mathbf{r}_0\}.$$

Let the basis vectors for $K_m(AM^{-1}, \mathbf{r}_0)$ and $K_m(M^{-H}A^H, \mathbf{r}_0)$ be $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m\}$ and $\{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_m\}$, the columns of V_m and W_m, respectively. The approximation to the solution of (1) at the mth QMR iteration is of the form

$$\mathbf{x}_m = \mathbf{x}_0 + M^{-1}V_m\mathbf{y}_m, \quad \mathbf{y}_m = \arg\min_{\mathbf{y}} \|\|\mathbf{r}_0\|\mathbf{e}_1 - T_{m+1,m}\mathbf{y}\|, \tag{3}$$

where $T_{m+1,m}$ is the $(m+1)\times m$ tridiagonal matrix of recurrence coefficients associated with two-sided Lanczos, namely,

$$T_{m+1,m} = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \gamma_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{m-1} \\ & & \gamma_{m-1} & \alpha_m \\ & & & \gamma_m \end{bmatrix};$$

see Algorithm 2.1 below. In (3) and throughout the paper the norm is the 2-norm.

By the construction of the two-sided Lanczos, the following relation holds:

$$AM^{-1}V_m = V_{m+1}T_{m+1,m}, \tag{4}$$

from which it follows that

$$\begin{aligned} \mathbf{r}_m &= \mathbf{b} - A\mathbf{x}_m \\ &= \mathbf{r}_0 - AM^{-1}V_m\mathbf{y}_m \qquad (5)\\ &= V_{m+1}(\|\mathbf{r}_0\|\mathbf{e}_1 - T_{m+1,m}\mathbf{y}_m). \qquad (6) \end{aligned}$$

This establishes that QMR produces the approximation $\mathbf{x}_m$ in such a way as to minimize the norm of the second factor of the residual (6); see (3). Thus, a quasi-minimization of the residual norm takes place. One can see from (5) that the residual at the mth step is of the form $\mathbf{r}_0 - AM^{-1}\mathbf{v}$ with $\mathbf{v} \in K_m(AM^{-1}, \mathbf{r}_0)$. Relation (4) can be rewritten

$$AZ_m^Q = V_{m+1}^Q T_{m+1,m}, \tag{7}$$

where $Z_m^Q = M^{-1}V_m$. We use superscripts Q and FQ to distinguish the vectors and matrices generated by QMR and FQMR, respectively. Correspondingly, rewriting (3), the approximate solution is of the form

$$\mathbf{x}_m = \mathbf{x}_0 + Z_m^Q\mathbf{y}_m, \quad \mathbf{y}_m = \arg\min_{\mathbf{y}} \|\|\mathbf{r}_0\|\mathbf{e}_1 - T_{m+1,m}\mathbf{y}\|.$$

Relation (4) illustrates that the action of AM^{-1} on a vector $\mathbf{v}$ of the Krylov subspace is in $K_{m+1}(AM^{-1}, \mathbf{r}_0)$ a basis of which are the columns of V_{m+1}^Q, while relation (7) will be useful in comparing QMR with FQMR. With this background in place, we present the following algorithm for FQMR.

Algorithm 2.1 (FQMR).

Given $\mathbf{x}_0$, form $\mathbf{r}_0$ and choose $\hat{\mathbf{r}}_0$ such that $\langle \mathbf{r}_0, \hat{\mathbf{r}}_0\rangle \neq 0$

set $\mathbf{v}_1 = \mathbf{r}_0/\|\mathbf{r}_0\|$ and $\mathbf{w}_1 = \hat{\mathbf{r}}_0/\langle \hat{\mathbf{r}}_0, \mathbf{v}_1\rangle$

set $\beta_0 = \gamma_0 = 0$ and $\mathbf{v}_0 = \mathbf{w}_0 = 0$

For $i = 1, 2, \ldots$

(8) Set $\mathbf{z}_i = M_i^{-1}\mathbf{v}_i$

$$\text{Compute: } A\mathbf{z}_i \text{ and } M_i^{-H}A^H\mathbf{w}_i \tag{9}$$
$$\alpha_i = \langle A\mathbf{z}_i, \mathbf{w}_i\rangle$$
$$\tilde{\mathbf{v}}_{i+1} = A\mathbf{z}_i - \alpha_i\mathbf{v}_i - \beta_{i-1}\mathbf{v}_{i-1} \tag{10}$$
$$\tilde{\mathbf{w}}_{i+1} = M_i^{-H}A^H\mathbf{w}_i - \bar{\alpha}_i\mathbf{w}_i - \gamma_{i-1}\mathbf{w}_{i-1}$$
$$\gamma_i = \|\tilde{\mathbf{v}}_{i+1}\|$$
$$\mathbf{v}_{i+1} = \tilde{\mathbf{v}}_{i+1}/\gamma_i \tag{11}$$
$$\beta_i = \langle \mathbf{v}_{i+1}, \tilde{\mathbf{w}}_{i+1}\rangle$$
$$\mathbf{w}_{i+1} = \tilde{\mathbf{w}}_{i+1}/\bar{\beta}_i$$
$$\mathbf{x}_i = \mathbf{x}_0 + Z_i^{FQ}\mathbf{y}_i, \quad \text{where } \mathbf{y}_i = \arg\min_{\mathbf{y}} \| \|\mathbf{r}_0\|\mathbf{e}_1 - T_{i+1,i}\mathbf{y}\| \text{ and } Z_i^{FQ} = [\mathbf{z}_1, \ldots, \mathbf{z}_i] \tag{12}$$

In this algorithm, $\bar{\alpha}_i$ and $\bar{\beta}_i$ stand for the conjugate of the complex numbers α_i and β_i, respectively. Note that the above algorithm represents a theoretical rendition of FQMR and not a full description of its implementation. In the actual implementation of FQMR the minimization in (12) is solved by performing a QR factorization of $T_{i+1,i}$. Using Givens rotations, this factorization of $T_{i+1,i}$ is easily updated from that of $T_{i,i-1}$, thus eliminating the need to save and construct $Z_i^{FQ} = [\mathbf{z}_1, \ldots, \mathbf{z}_i]$ at each step.

If we replace M_i with M, a fixed preconditioner, the above algorithm reduces to the standard QMR method. Thus, implementation of FQMR requires only a slight modification of the code for QMR, and this is one of the strengths of this new algorithm.

Let us discuss the variable preconditioned step (8) in some detail. If the preconditioned equations $M\mathbf{z} = \mathbf{v}$ are solved approximately by a second iterative solver, then we can write (8) in terms of M^{-1} and $\boldsymbol{\varepsilon}_i$, where $\boldsymbol{\varepsilon}_i$ is the error associated with the inner solve at step i. Thus, for this case we write

$$\mathbf{z}_i = M_i^{-1}\mathbf{v}_i = M^{-1}\mathbf{v}_i + \boldsymbol{\varepsilon}_i. \tag{13}$$

This description of flexible preconditioning is used in [16] for investigating inexact conjugate gradient.

A consequence of flexible preconditioning is the relation

$$AZ_m^{FQ} = V_{m+1}^{FQ}T_{m+1,m}, \tag{14}$$

where Z_m^{FQ} is the matrix whose ith column is $\mathbf{z}_i$, the vector constructed by FQMR in (8); cf. (7). Let us denote by $\hat{K}_m$ the subspace spanned by the columns of Z_m^{FQ}, which, in general, is not a Krylov subspace. Consequently, relation (14) cannot be simplified into a form similar to relation (4) since the action AM_i^{-1} on a vector $\mathbf{v}$ of the Krylov subspace is no longer in the span of the columns of V_{m+1}. Using (14), however, we can still display a quasi-minimization property held by $\mathbf{x}_m$ over this new $\hat{K}_m$, and this is why the convergence theory in [9] applies to FQMR. The proof is identical to the one for QMR as we show in what follows. For an arbitrary vector in the space $\mathbf{x}_0 + \hat{K}_m$, i.e., of the form $\mathbf{z} = \mathbf{x}_0 + Z_m^{FQ}\mathbf{y}$, for some $\mathbf{y} \in \mathbb{C}^m$, we have the following identities

$$\begin{aligned}\mathbf{b} - A\mathbf{z} = \mathbf{b} - A(\mathbf{x}_0 + Z_m^{FQ}\mathbf{y}) \ &= \ \mathbf{r}_0 - AZ_m^{FQ}\mathbf{y} \\ &= V_{m+1}^{FQ}(\|r_0\|\mathbf{e}_1 - T_{m+1,m}\mathbf{y}).\end{aligned}$$

Now, since $\mathbf{x}_m$ is chosen to minimize the norm of $\|r_0\|\mathbf{e}_1 - T_{m+1,m}\mathbf{y}$, we see that FQMR maintains the quasi-minimal residual property over the affine space $\mathbf{x}_0 + \hat{K}_m$.

We remark that FQMR with left preconditioning does not follow an analogous construction. For flexible left preconditioning, relation (14) no longer holds, and therefore $\mathbf{x}_i$ cannot be updated as in (12).

Another noteworthy observation is that FQMR, by construction, maintains the three-term recurrence of QMR. However, in so doing, there is a loss of the global biorthogonality held by the bases generated by QMR. However, a local biorthogonality property is maintained, as shown in the following theorem. That is, consecutive Lanczos vectors constructed by the flexible two-sided Lanczos process are biorthogonal. We note, however, that for the results of this theorem to hold, we are assuming that at each step of the outer iteration the matrix M_i is the same matrix used in (8) and in (9). Theoretically this is a logical assumption, and in some cases this is also true in practice, but in general this assumption does not necessarily hold.

THEOREM 2.2. *If the two-sided Lanczos vectors are defined at steps* $1, \ldots, k+1$ *in Algorithm* 2.1*, i.e., if* $\langle \mathbf{v}_i, \mathbf{w}_i \rangle \neq 0$ *for* $i = 1, \ldots, k+1$*, then*

$$\langle \mathbf{v}_{k+1}, \mathbf{w}_k \rangle = 0 \quad \textit{and} \quad \langle \mathbf{w}_{k+1}, \mathbf{v}_k \rangle = 0. \tag{15}$$

Proof. We first note that $\|\mathbf{v}_i\| = 1$ for all i by the choice of γ_{i-1}. Likewise $\langle \mathbf{v}_i, \mathbf{w}_i \rangle = 1$ for all i by the choice of γ_{i-1} and $\bar{\beta}_{i-1}$. We prove (15) by induction. For $k = 0$ the result is obvious since $\mathbf{v}_0 = \mathbf{w}_0 = 0$. Assume that (15) holds for $i \leq k-1$; then

$$\begin{aligned}
\langle \tilde{\mathbf{v}}_{k+1}, \mathbf{w}_k \rangle &= \langle AM_k^{-1}\mathbf{v}_k, \mathbf{w_k} \rangle - \alpha_k \langle \mathbf{v}_k, \mathbf{w}_k \rangle - \beta_{k-1} \langle \mathbf{v}_{k-1}, \mathbf{w}_k \rangle \\
&= \langle AM_k^{-1}\mathbf{v}_k, \mathbf{w_k} \rangle - \alpha_k = 0
\end{aligned}$$

and

$$\begin{aligned}
\langle \tilde{\mathbf{w}}_{k+1}, \mathbf{v}_k \rangle &= \langle M_k^{-H} A^H \mathbf{w}_k, \mathbf{v}_k \rangle - \bar{\alpha}_k \\
&= \langle M_k^{-H} A^H \mathbf{w}_k, \mathbf{v}_k \rangle - \overline{\langle AM_k^{-1}\mathbf{v}_k, \mathbf{w}_k \rangle} \\
&= \langle M_k^{-H} A^H \mathbf{w}_k, \mathbf{v}_k \rangle - \overline{\langle \mathbf{v}_k, M_k^{-H} A^H \mathbf{w}_k \rangle} = 0. \qquad \square
\end{aligned}$$

3. FQMR and FGMRES.

Generalized minimal residual (GMRES) [23] is another successful Krylov subspace method for solving non-Hermitian systems of linear equations. Like QMR, GMRES can be implemented with a flexible preconditioner, and the flexible version is called FGMRES [21]. In this section we establish a relationship between FQMR and FGMRES which is reminiscent of a relationship held by QMR and GMRES [19]. As a precursor to the statement of this relationship, we give a brief summary of GMRES with a fixed right preconditioner; see [17], [22], or [23] for a full description.

At the mth iteration, preconditioned GMRES produces an approximation $\mathbf{x}_m$ to the solution of (1) in $\mathbf{x}_0 + K_m(AM^{-1}, \mathbf{r}_0)$ in such a way as to minimize the norm of the residual over $K_m(AM^{-1}, \mathbf{r}_0)$, i.e.,

$$\mathbf{x}_m = \mathbf{x}_0 + \arg \min_{\mathbf{z} \in K_m(AM^{-1}, \mathbf{r}_0)} \| \mathbf{r}_0 - AM^{-1}\mathbf{z} \|.$$

This minimization is accomplished by constructing an orthonormal basis for $K_m(AM^{-1}, \mathbf{r}_0)$ using the Arnoldi method [17]. In the Arnoldi method the basis vectors, $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m\}$, are formed recursively by orthogonalizing a new vector, $\hat{\mathbf{v}}_{i+1}$, in $K_{i+1}(AM^{-1}, \|\mathbf{r}_0\|)$ against the previous vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_i$ in $K_i(AM^{-1}, \|\mathbf{r}_0\|)$ and then normalizing it, so that $\mathbf{v}_{i+1} = \hat{\mathbf{v}}_{i+1}/\|\hat{\mathbf{v}}_{i+1}\|$. Thus,

$$\mathbf{v}_{i+1} = \frac{1}{h_{i+1,i}} \left(AM^{-1}\mathbf{v}_i - \sum_{k=1}^{i} h_{k,i}\mathbf{v}_k \right), \tag{16}$$

where the coefficients $h_{k,i},\ k = 1, \ldots, i+1$, are appropriately chosen to orthogonalize and normalize $\mathbf{v}_{i+1}$. From (16) we get the relation

$$AM^{-1}V_m = V_{m+1}H_{m+1,m}, \tag{17}$$

where $H_{m+1,m}$ is the upper-Hessenberg matrix whose nonzero entries are the coefficients $h_{k,i},\ k = 1, \ldots, i+1$, from (16), $i = 1, \ldots, m$.

With this groundwork in place, we can now establish that GMRES computes the approximation $\mathbf{x}_m = \mathbf{x}_0 + V_m\mathbf{y}_m$ such that

$$\begin{aligned} \mathbf{y}_m &= \arg\min_{\mathbf{y}} \|\mathbf{r}_0 - AM^{-1}V_m\mathbf{y}\| = \arg\min_{\mathbf{y}} \|\mathbf{r}_0 - V_{m+1}H_{m+1,m}\mathbf{y}\| \\ &= \arg\min_{\mathbf{y}} \|\|\mathbf{r}_0\|\mathbf{e}_1 - H_{m+1,m}\mathbf{y}\|. \end{aligned} \tag{18}$$

Observe that while in (3) QMR only minimizes the norm of a factor of the residual, in (18) we have that GMRES minimizes the norm of the actual residual, since V_{m+1} is unitary.

We end this introduction of GMRES by pointing out that when the preconditioner changes from step to step, i.e., when one uses M_i instead of M in (16), we have FGMRES [21]. In what follows, we use superscripts G and FG to distinguish the vectors and matrices generated by GMRES and FGMRES, respectively.

Let $\mathbf{z}_i = M_i^{-1}\mathbf{v}_i$, and let Z_m^{FG} be the matrix with columns $\mathbf{z}_1, \ldots, \mathbf{z}_m$; then the following relation analogous to (17) holds for FGMRES:

$$AZ_m^{FG} = V_{m+1}^{FG}H_{m+1,m}. \tag{19}$$

When QMR and GMRES are implemented with fixed preconditioning, we have the following result due to Nachtigal [19], where κ_2 denotes the condition number using the 2-norm; see also [17], [22].

THEOREM 3.1. *If $\mathbf{r}_m^G$ denotes the GMRES residual at step m and $\mathbf{r}_m^Q$ denotes the QMR residual at step m, then*

$$\|\mathbf{r}_m^Q\| \leq \kappa_2(V_{m+1}^Q)\|\mathbf{r}_m^G\|, \tag{20}$$

where V_{m+1}^Q is the matrix whose columns are the basis vectors generated by QMR.

This inequality works out nicely since V_{m+1}^G constructed by GMRES and V_{m+1}^Q constructed by QMR are both a basis for the same Krylov subspace. When flexible preconditioning is used, this is no longer the case. To avoid confusion, let us denote by $\mathbf{v}_{i+1}^{FQ}$ and $\mathbf{v}_{i+1}^{FG}$ the vectors computed by FQMR in (11) and by FGMRES in (16), respectively. We can, however, prove a relation similar to (20) for FGMRES and FQMR, but to do so we first need the following lemma relating Z_m^{FG} and Z_m^{FQ}, the basis of the subspaces constructed by FGMRES and FQMR, respectively; see (19) and (14).

LEMMA 3.2. *Let $\mathbf{z}_i^{FG}$ be the ith column of Z_m^{FG} satisfying* (19). *Likewise, let $\mathbf{z}_i^{FQ}$ be the ith column of Z_m^{FQ} satisfying* (14). *If $\boldsymbol{\varepsilon}_i^{FQ}$ is the ith error vector defined by*

$$\mathbf{z}_i^{FQ} = M^{-1}\mathbf{v}_i^{FQ} + \boldsymbol{\varepsilon}_i^{FQ} \tag{21}$$

and if $\boldsymbol{\varepsilon}_i^{FG}$ is the ith error vector defined by

$$\mathbf{z}_i^{FG} = M^{-1}\mathbf{v}_i^{FG} + \boldsymbol{\varepsilon}_i^{FG}, \tag{22}$$

then

$$\mathbf{z}_i^{FG} \in S^m, \quad i = 1, \ldots, m, \tag{23}$$

where

$$S^m = \operatorname{span}\{\mathbf{z}_i^{FQ}, (M^{-1}A)^j \boldsymbol{\varepsilon}_i^{FQ}, (M^{-1}A)^j \boldsymbol{\varepsilon}_i^{FG};\ i = 1, \ldots, m,\ j = 0, \ldots, m-1\}.$$

Proof. We show (23) by induction on m. For $m = 1$, since $\mathbf{v}_1^{FG} = \mathbf{v}_1^{FQ} = \mathbf{r}_0/\|\mathbf{r}_0\|$, we have $\mathbf{z}_1^{FG} = M^{-1}\mathbf{v}_1^{FG} + \boldsymbol{\varepsilon}_1^{FG} = M^{-1}\mathbf{v}_1^{FQ} + \boldsymbol{\varepsilon}_1^{FG} = \mathbf{z}_1^{FQ} - \boldsymbol{\varepsilon}_1^{FQ} + \boldsymbol{\varepsilon}_1^{FG} \in S^1$. Assuming that (23) holds for $n \le m$, then

$$\begin{aligned}
\mathbf{z}_{m+1}^{FG} &= M^{-1}\mathbf{v}_{m+1}^{FG} + \boldsymbol{\varepsilon}_{m+1}^{FG} \\
&= M^{-1}\left(\tfrac{1}{h_{m+1,m}}\right)\left(Az_m^{FG} - \sum_{k=1}^{m} h_{k,m}\mathbf{v}_k^{FG}\right) + \boldsymbol{\varepsilon}_{m+1}^{FG} \\
&= \left(\tfrac{1}{h_{m+1,m}}\right)\left(M^{-1}A\mathbf{z}_m^{FG} - \sum_{k=1}^{m} h_{k,m}M^{-1}\mathbf{v}_k^{FG} + h_{m+1,m}\boldsymbol{\varepsilon}_{m+1}^{FG}\right) \\
&= \left(\tfrac{1}{h_{m+1,m}}\right)\left(M^{-1}A\mathbf{z}_m^{FG} - \sum_{k=1}^{m} (h_{k,m}\mathbf{z}_k^{FG} - h_{k,m}\boldsymbol{\varepsilon}_k^{FG}) + h_{m+1,m}\boldsymbol{\varepsilon}_{m+1}^{FG}\right),
\end{aligned}$$

where the first and last equalities follow from (22) and the second equality follows from the definition of $\mathbf{v}_{m+1}^{FG}$.

By the induction hypothesis and the observation that $S^r \subseteq S^t$ for $r \le t$, we have that $\mathbf{z}_i^{FG} \in S^{m+1}$ for $i \le m$. By the definition of S^{m+1}, $\boldsymbol{\varepsilon}_i^{FG} \in S^{m+1}$ for $i \le m+1$. Therefore, all that remains to be shown is that the first term $M^{-1}A\mathbf{z}_m^{FG} \in S^{m+1}$. Again by the induction hypothesis, we know that $\mathbf{z}_m^{FG} \in S^m$; hence, there are scalars $a_i, b_{i,j}, c_{i,j},\ i = 1, \ldots m,\ j = 0, \ldots, m-1$, such that

$$\mathbf{z}_m^{FG} = \sum_{i=1}^{m} a_i \mathbf{z}_i^{FQ} + \sum_{k=0}^{m-1}\left(\sum_{i=1}^{m} b_{i,k}(M^{-1}A)^k \boldsymbol{\varepsilon}_i^{FQ}\right) + \sum_{k=0}^{m-1}\left(\sum_{i=1}^{m} c_{i,k}(M^{-1}A)^k \boldsymbol{\varepsilon}_i^{FG}\right),$$

and therefore

$$\begin{aligned}
M^{-1}A\mathbf{z}_m^{FG} = \sum_{i=1}^{m} a_i (M^{-1}A)\mathbf{z}_i^{FQ} &+ \sum_{k=0}^{m-1}\left(\sum_{i=1}^{m} b_{i,k}(M^{-1}A)^{k+1} \boldsymbol{\varepsilon}_i^{FQ}\right) \\
&+ \sum_{k=0}^{m-1}\left(\sum_{i=1}^{m} c_{i,k}(M^{-1}A)^{k+1} \boldsymbol{\varepsilon}_i^{FG}\right).
\end{aligned}$$

Since $(M^{-1}A)^j \boldsymbol{\varepsilon}_i^{FG} \in S^{m+1}$ and $(M^{-1}A)^j \boldsymbol{\varepsilon}_i^{FQ} \in S^{m+1}$ for $j = 0, \ldots, (m+1)-1$, $i = 1, \ldots, m+1$ by definition of S^{m+1}, all that remains to be shown is $(M^{-1}A)\mathbf{z}_i^{FQ} \in S^{m+1}$ for $i = 1, \ldots, m$. Solving in (10) for $A\mathbf{z}_j$ and multiplying through by M^{-1} gives

$$(M^{-1}A)\mathbf{z}_i^{FQ} = \gamma_i M^{-1}\mathbf{v}_{i+1}^{FQ} + \alpha_i M^{-1}\mathbf{v}_i^{FQ} + \beta_{i-1}M^{-1}\mathbf{v}_{i-1}^{FQ}. \tag{24}$$

Next, solving (21) for $M^{-1}\mathbf{v}_i^{FQ}$ and substituting this into (24) gives

$$(M^{-1}A)\mathbf{z}_i^{FQ} = \gamma_i\mathbf{z}_{i+1}^{FQ} - \gamma_i\boldsymbol{\varepsilon}_{i+1}^{FQ} + \alpha_i\mathbf{z}_i^{FQ} - \alpha_i\boldsymbol{\varepsilon}_i^{FQ} + \beta_{i-1}\mathbf{z}_{i-1}^{FQ} - \beta_{i-1}\boldsymbol{\varepsilon}_{i-1}^{FQ} \in S^{m+1}. \qquad \square \tag{25}$$

We can now prove our main result.

THEOREM 3.3. *Assume that V_{m+1}^{FQ}, the matrix satisfying* (14), *is of full rank. Let $\mathbf{r}_m^{FQ}$ and $\mathbf{r}_m^{FG}$ be the residuals obtained after m steps of the FQMR and FGMRES algorithms, respectively, and let $\mathcal{E}_m^{FQ} = [\boldsymbol{\varepsilon}_1^{FQ}, \ldots, \boldsymbol{\varepsilon}_m^{FQ}]$ and $\mathcal{E}_m^{FG} = [\boldsymbol{\varepsilon}_1^{FG}, \ldots, \boldsymbol{\varepsilon}_m^{FG}]$, where $\boldsymbol{\varepsilon}_i^{FQ}$ and $\boldsymbol{\varepsilon}_i^{FG}$ are the error vectors in* (21) *and* (22)*, respectively. Then there exist vectors $\mathbf{y}_k^{FQ}, \mathbf{y}_k^{FG} \in \mathbb{R}^m$, $k = 1, \ldots, m-1$, such that the following holds:*

$$\|\mathbf{r}_m^{FQ}\| \le \kappa_2(V_{m+1}^{FQ}) \left[\|\mathbf{r}_m^{FG}\| + \sum_{k=0}^{m-1} \|A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}\| + \sum_{k=0}^{m-1} \|A(M^{-1}A)^k \mathcal{E}_m^{FG}\mathbf{y}_k^{FG}\| \right].$$

Proof. Step 1. Consider the set defined by

$$\mathcal{R} = \{\mathbf{r} : \ \mathbf{r} = V_{m+1}^{FQ}\mathbf{t}; \ \mathbf{t} = \beta\mathbf{e}_1 - T_{m+1,m}\mathbf{y}; \ \mathbf{y} \in \mathbb{C}^m\}.$$

Let $\mathbf{y}_m$ denote the vector $\mathbf{y}$ that minimizes $\|\beta e_1 - T_{m+1,m}\mathbf{y}\|$, and denote by $\mathbf{t}_m = \beta e_1 - T_{m+1,1}\mathbf{y}_m$. Then by definition we have $\mathbf{r}_m^{FQ} = V_{m+1}^{FQ}\mathbf{t_m}$. By hypothesis, V_{m+1}^{FQ} is of full rank. Therefore, there is an $(m+1)\times(m+1)$ nonsingular matrix S such that $W_{m+1} = V_{m+1}^{FQ}S$ is unitary. Then for any element of the set $\mathcal{R}$,

$$\mathbf{r} = W_{m+1}S^{-1}\mathbf{t}\ , \qquad \mathbf{t} = SW_{m+1}^H\mathbf{r},$$

and, in particular, $\mathbf{r}_m^{FQ} = W_{m+1}S^{-1}\mathbf{t}_m$, which implies

$$\|\mathbf{r}_m^{FQ}\| \le \|S^{-1}\|\|\mathbf{t}_m\|. \tag{26}$$

From (3), it follows that the norm $\|\mathbf{t}_m\|$ is the minimum of $\|\beta e_1 - T_{m+1,m}\mathbf{y}\|$ over all vectors $\mathbf{y}$, and therefore

$$\|\mathbf{t}_m\| = \|SW_{m+1}^H\mathbf{r}_m^{FQ}\| \le \|SW_{m+1}^H\mathbf{r}\| \le \|S\|\|\mathbf{r}\| \quad \text{for all } \mathbf{r} \in \mathcal{R}. \tag{27}$$

Step 2. We now consider

$$\mathbf{r}_m^{FG} = \mathbf{r}_0 - AZ_m^{FG}\mathbf{y}_m^{FG}, \qquad \text{where } \mathbf{y}_m^{FG} \text{ minimizes } \|\mathbf{r}_0 - AZ_m^{FG}\mathbf{y}\|. \tag{28}$$

By Lemma 3.2 there exists vectors $\mathbf{y}_z$, $\mathbf{y}_k^{FQ}$, $\mathbf{y}_k^{FG} \in \mathbb{R}^m$; $k = 0, \ldots, m-1$, such that

$$\begin{aligned}
\mathbf{r}_m^{FG} &= \mathbf{r}_0 - AZ_m^{FQ}\mathbf{y}_z - \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ} - \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FG}\mathbf{y}_k^{FG} \\
&= \mathbf{r}_0 - V_{m+1}^{FQ}T_{m+1,m}\mathbf{y}_z - \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ} - \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FG}\mathbf{y}_k^{FG}.
\end{aligned}$$

By rearrangement of terms,

$$\mathbf{r}_0 - V_{m+1}^{FQ}T_{m+1,m}\mathbf{y}_z = \mathbf{r}_m^{FG} + \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ} + \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FG}\mathbf{y}_k^{FG}.$$

Let $\hat{\mathbf{r}} = V_{m+1}^{FQ}(\|\mathbf{r}_0\|e_1 - T_{m+1,m}\mathbf{y}_z)$; then

$$\begin{aligned}\|\hat{\mathbf{r}}\| &= \|V_{m+1}^{FQ}(\|\mathbf{r}_0\|\mathbf{e}_1 - T_{m+1,m}\mathbf{y}_z)\| = \|\mathbf{r}_0 - V_{m+1}^{FQ}T_{m+1,m}\mathbf{y}_z\| \\ &\le \|\mathbf{r}_m^{FG}\| + \sum_{k=0}^{m-1}\|A(M^{-1}A)^k\mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}\| + \sum_{k=0}^{m-1}\|A(M^{-1}A)^k\mathcal{E}_m^{FG}\mathbf{y}_k^{FG}\|. \end{aligned} \tag{29}$$

Since $\hat{\mathbf{r}} \in \mathcal{R}$, by (27),

$$\|\mathbf{t}_m\| \le \|S\|\|\hat{\mathbf{r}}\|. \tag{30}$$

Hence, by (26), (29), and (27),

$$\begin{aligned}\|\mathbf{r}_m^{FQ}\| &\le \|S^{-1}\|\|\mathbf{t}_m\| \\ &\le \|S^{-1}\|\|S\|\left[\|\mathbf{r}_m^{FG}\| + \sum_{k=0}^{m-1}\|A(M^{-1}A)^k\mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}\| + \sum_{k=0}^{m-1}\|A(M^{-1}A)^k\mathcal{E}_m^{FG}\mathbf{y}_k^{FG}\|\right]\end{aligned}$$

and since $\kappa_2(V_{m+1}^{FQ}) = \kappa_2(S) = \|S^{-1}\|\|S\|$, the theorem follows. □

We comment that as $\boldsymbol{\varepsilon}_i$ goes to $\mathbf{0}$, the bound on $\|\mathbf{r}_m^{FQ}\|$ in Theorem 3.3 is reduced. However, we cannot know how sharp this bound is due to the existence of vectors $\mathbf{y}_k^{FQ}, \mathbf{y}_k^{FG}$ in the right-hand side of the inequality.

By considering exact solutions of the preconditioned equations (13), i.e., if $\boldsymbol{\varepsilon}_i = 0$ in (13), or equivalently if $M_i = M$ for all i, then FQMR and FGMRES are reduced to QMR and GMRES with fixed preconditioners and Theorem 3.3 reduces to Theorem 3.1. There are two other special situations, which we want to highlight. If $\mathcal{E}_m^{FG} = 0$, i.e., $\boldsymbol{\varepsilon}_i^{FQ} = 0$ for all i, then FGMRES reduces to GMRES, and we have the following corollary.

Corollary 3.4. *Let V_{m+1}^{FQ}, $\mathcal{E}_m^{FQ}$, and $\mathbf{r}_m^{FQ}$ be as described in Theorem 3.3, and let $\mathbf{r}_m^{G}$ be the residual obtained after m steps of the GMRES algorithm. Then there exists vectors $\mathbf{y}_k^{FQ} \in \mathbb{R}^m$, $k = 1, \ldots, m-1$, such that the following holds:*

$$\|\mathbf{r}_m^{FQ}\| \le \kappa_2(V_{m+1}^{FQ})\left(\|\mathbf{r}_m^{G}\| + \sum_{k=0}^{m-1}\|A(M^{-1}A)^k\mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}\|\right).$$

Likewise, if $\mathcal{E}_m^{FQ} = 0$, i.e., $\boldsymbol{\varepsilon}_i^{FQ} = 0$ for all i, then the following corollary, which is a new result for FGMRES, is also established.

Corollary 3.5. *Let V_{m+1}^{Q}, $\mathcal{E}_m^{FG}$, and $\mathbf{r}_m^{FG}$ be as described in Theorems 3.1 and 3.3, and let $\mathbf{r}_m^{Q}$ be the residual obtained after m steps of the QMR algorithm. Then there exists vectors $\mathbf{y}_k^{FG} \in \mathbb{R}^m$, $k = 1, \ldots, m-1$, such that the following holds:*

$$\|\mathbf{r}_m^{Q}\| \le \kappa_2(V_{m+1}^{Q})\left(\|\mathbf{r}_m^{FG}\| + \sum_{k=0}^{m-1}\|A(M^{-1}A)^k\mathcal{E}_m^{FG}\mathbf{y}_k^{FG}\|\right).$$

We end this section with a comment on the hypothesis in Theorem 3.3 that V_{m+1}^{FQ} be of full rank. This implies that the subspace $\hat{K}_m$ has dimension m, i.e., that at each step we are minimizing over increasingly larger subspaces. Note that this hypothesis implies that the subspaces $\hat{K}_m$ are nested, and this is precisely the assumption made in [9] for the convergence proofs.

4. Bounds on residual norms. Using the same techniques used in Lemma 3.2 and Theorem 3.3, we provide bounds on the norm of the residual of FQMR in terms of the norm of the residual of QMR. The following lemma relates Z_m^{FQ} to Z_m^Q, the matrices whose columns are the basis of the subspaces generated by FQMR and QMR, respectively; see (14) and (7). We first establish an auxiliary lemma.

LEMMA 4.1. *Let $\mathbf{z}_i^{FQ}$ be the ith column of Z_m^{FQ}, and let $\mathbf{z}_i^Q$ be the ith column of Z_m^Q. If $\boldsymbol{\varepsilon}_i^{FQ}$ is the ith error vector defined by* (21)*, then*

$$\mathbf{z}_i^Q \in S^m, \quad i = 1, \ldots, m, \tag{31}$$

where $S^m = \operatorname{span}\{\mathbf{z}_i^{FQ}, (M^{-1}A)^j \boldsymbol{\varepsilon}_i^{FQ};\ i = 1, \ldots, m,\ j = 0, \ldots, m-1\}$.

Proof. We show (31) by induction on m. For $m = 1$, we have $\mathbf{z}_1^Q = M^{-1}\mathbf{v}_1^Q = M^{-1}\mathbf{v}_1^{FQ} = \mathbf{z}_1^{FQ} - \boldsymbol{\varepsilon}_1^{FQ} \in S^1$. Assuming that (31) holds for $n \le m$, then

$$\begin{aligned}
\mathbf{z}_{m+1}^Q &= M^{-1}\mathbf{v}_{m+1}^Q \\
&= M^{-1}(\tfrac{1}{\gamma_m})(A\mathbf{z}_m^Q - \alpha_m \mathbf{v}_m^Q - \beta_{m-1}\mathbf{v}_{m-1}^Q) \\
&= (\tfrac{1}{\gamma_m})(M^{-1}A\mathbf{z}_m^Q - \alpha_m M^{-1}\mathbf{v}_m^Q - \beta_{m-1}M^{-1}\mathbf{v}_{m-1}^Q) \\
&= (\tfrac{1}{\gamma_m})(M^{-1}A\mathbf{z}_m^Q - \alpha_m \mathbf{z}_m^Q - \beta_{m-1}\mathbf{z}_{m-1}^Q),
\end{aligned}$$

where the first and last equalities follow from the relation (2), and the second equality follows from the definition of $\mathbf{v}_{m+1}^Q$; see (10). By the induction hypothesis and the observation that $S^r \subseteq S^t$ for $r \le t$, we have that $\mathbf{z}_i^Q \in S^{m+1}$ for $i \le m$. Therefore, all that remains to be shown is that $M^{-1}A\mathbf{z}_m^Q \in S^{m+1}$. Again by the induction hypothesis, we know that $\mathbf{z}_m^Q \in S^m$; hence, there are scalars $a_i, b_{i,j},\ i = 1, \ldots m,\ j = 0, \ldots, m-1$, such that

$$\mathbf{z}_m^Q = \sum_{i=1}^{m} a_i \mathbf{z}_i^{FQ} + \sum_{k=0}^{m-1} \left(\sum_{i=1}^{m} b_{i,k} (M^{-1}A)^k \boldsymbol{\varepsilon}_i^{FQ} \right),$$

and therefore

$$M^{-1}A\mathbf{z}_m^Q = \sum_{i=1}^{m} a_i (M^{-1}A)\mathbf{z}_i^{FQ} + \sum_{k=0}^{m-1} \left(\sum_{i=1}^{m} b_{i,k} (M^{-1}A)^{k+1} \boldsymbol{\varepsilon}_i^{FQ} \right).$$

Since $(M^{-1}A)^j \boldsymbol{\varepsilon}_i^{FQ} \in S^{m+1}$ for $j = 0, \ldots, (m+1)-1,\ i = 1, \ldots, m+1$, all that remains to show is $(M^{-1}A)\mathbf{z}_i^{FQ} \in S^{m+1}$ for $i = 1, \ldots, m$, but this follows from (25). ∎

Using Lemma 4.1, we now present the following theorem.

THEOREM 4.2. *Assume that V_{m+1}^{FQ}, the matrix satisfying* (14)*, is of full rank. Let $\mathbf{r}_m^{FQ}$ and $\mathbf{r}_m^Q$ be the residuals obtained after m steps of the FQMR and QMR algorithms, respectively, and let $\mathcal{E}_m^{FQ} = [\boldsymbol{\varepsilon}_1^{FQ}, \ldots, \boldsymbol{\varepsilon}_m^{FQ}]$, where $\boldsymbol{\varepsilon}_i^{FQ}$ are the error vectors defined by* (21)*. Then there exists vectors $\mathbf{y}_k^{FQ} \in \mathbb{R}^m$, $k = 1, \ldots, m-1$, such that the following holds:*

$$\|\mathbf{r}_m^{FQ}\| \le \kappa_2(V_{m+1}^{FQ}) \left(\|\mathbf{r}_m^Q\| + \sum_{k=0}^{m-1} \|A(M^{-1}A)^k \mathcal{E}_m^{FQ} \mathbf{y}_k^{FQ}\| \right).$$

Proof. Step 1 of the proof is identical to Step 1 of the proof of Theorem 3.3.

Step 2. Consider

$$\mathbf{r}_m^Q = \mathbf{r}_0 - AZ_m^Q\mathbf{y}_m^Q, \quad \text{where } \mathbf{y}_m^Q \text{ minimizes } \|\mathbf{r}_0 - AZ_m^Q\mathbf{y}\|. \tag{32}$$

By Lemma 4.1 there exists vectors $\mathbf{y}_z,\ \mathbf{y}_k^{FQ},\ k = 0, \ldots, m-1$, such that

$$\begin{aligned}\mathbf{r}_m^Q &= \mathbf{r}_0 - AZ_m^{FQ}\mathbf{y}_z - \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ} \\ &= \mathbf{r}_0 - V_{m+1}^{FQ}T_{m+1,m}\mathbf{y}_z - \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}.\end{aligned}$$

By rearrangement of terms,

$$\mathbf{r}_0 - V_{m+1}^{FQ}T_{m+1,m}\mathbf{y}_z = \mathbf{r}_m^Q + \sum_{k=0}^{m-1} A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}.$$

Let $\hat{\mathbf{r}} = V_{m+1}^{FQ}(\|\mathbf{r}_0\|\mathbf{e}_1 - T_{m+1,m}\mathbf{y}_z) = \mathbf{r}_0 - V_{m+1}^{FQ}T_{m+1,m}\mathbf{y}_z$; then

$$\|\hat{\mathbf{r}}\| \le \|\mathbf{r}_m^Q\| + \sum_{k=0}^{m-1} \|A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}\|.$$

Since $\hat{\mathbf{r}} \in \mathcal{R}$, by (27)

$$\|\mathbf{t}_m\| \le \|S\|\|\hat{\mathbf{r}}\|. \tag{33}$$

Hence, by (26) and (33) we obtain

$$\|\mathbf{r}_m^{FQ}\| \le \|S^{-1}\|\|\mathbf{t}_m\| \le \|S^{-1}\|\|S\| \left(\|\mathbf{r}_m^Q\| + \sum_{k=0}^{m-1} \|A(M^{-1}A)^k \mathcal{E}_m^{FQ}\mathbf{y}_k^{FQ}\|\right),$$

and since $\kappa_2(V_{m+1}^{FQ}) = \kappa_2(S) = \|S^{-1}\|\|S\|$, the theorem follows. □

Using identical techniques as in Lemma 4.1 and Theorem 4.2 one can prove the following new result relating the norm of the residuals associated with GMRES and FGMRES.

THEOREM 4.3. *Assume that V_{m+1}^{FG}, the matrix satisfying* (19), *is of full rank. Let $\mathbf{r}_m^{FG}$ and $\mathbf{r}_m^G$ be the residuals obtained after m steps of the FGMRES and GMRES algorithms, respectively, and let $\mathcal{E}_m^{FG} = [\boldsymbol{\varepsilon}_1^{FG}, \ldots, \boldsymbol{\varepsilon}_m^{FG}]$, where $\boldsymbol{\varepsilon}_i^{FG}$ are the ith error vectors given by* (22). *Then there exists vectors $\mathbf{y}_k^{FG} \in \mathbb{R}^m$, $k = 1, \ldots, m-1$, such that the following holds:*

$$\|\mathbf{r}_m^{FG}\| \le \kappa_2(V_{m+1}^{FG}) \left(\|\mathbf{r}_m^G\| + \sum_{k=0}^{m-1} \|A(M^{-1}A)^k \mathcal{E}_m^{FG}\mathbf{y}_k^{FG}\|\right).$$

5. Numerical experiments.

To illustrate the behavior of FQMR we performed several numerical experiments. We begin by considering a set of examples from [21] given by a finite difference discretization of the partial differential equation

$$-\Delta u + \gamma(xu_x + yu_y) + \beta u = f \tag{34}$$

on a unit square, where f is such that the exact solution to the discretized equation $A\mathbf{x} = \mathbf{b}$ is $\mathbf{x}^H = (1, \ldots, 1)$. The parameters γ and β are chosen in one case to make the system indefinite ($\gamma = 10$ and $\beta = -100$) and in another to have a highly nonsymmetric matrix ($\gamma = 1000$ and $\beta = 10$). For $\gamma \neq 0$, A is non-Hermitian, and it is appropriate to use FQMR. The mesh is chosen as in [21] of equal size in both dimensions (32 nodes), and the corresponding matrix is thus of order 1024.

In our experiments, we ran FQMR preconditioned with the standard QMR method (FQMR-QMR), FQMR preconditioned with QMR which, in turn, is preconditioned with ILU(0) (FQMR-QMR(ILU(0))), and FQMR preconditioned with CGNE (FQMR-CGNE); see, e.g., [17], [22] for descriptions of these preconditioners. When possible, each of these was run with an outer relative residual norm tolerance of 10^{-7} and an inner relative residual tolerance ranging from 10^{-1} to 10^{-6}. In all of our experiments, our stopping criteria uses the 2-norm in computing the relative residual norm $\|\mathbf{r}_k\|/\|r_0\|$, which is consistent with our theoretical analysis. Our FORTRAN code is derived from the existing code for QMR taken from [12], and ILU(0) and CGNE are taken from [3]. Our experiments were run on a DEC-alpha machine; however, for easy comparisons with runs on other machines, in our tables and figures we report number of operations and not computer times. The trends observed in our tables and figures are very similar to those one would observe using CPU times.

Table 1
FQMR-QMR. $\beta = -100, \gamma = 10$, *out. tol.* $= 10^{-7}$.

Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-1}	15	97	1.70×10^8
10^{-2}	5	110	6.47×10^7
10^{-3}	3	124	4.35×10^7
10^{-4}	2	131	$\mathbf{3.06\times10^7}$
10^{-5}	2	158	3.70×10^7
10^{-6}	2	183	4.28×10^7

Table 2
FQMR-QMR. $\beta = 10, \gamma = 1000$, *out. tol.* $= 10^{-7}$.

Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-1}	10	122	1.43×10^8
10^{-2}	4	149	7.00×10^7
10^{-3}	3	171	6.02×10^7
10^{-4}	2	204	$\mathbf{4.77\times10^7}$
10^{-5}	2	230	5.39×10^7
10^{-6}	2	248	5.80×10^7

Tables 1 and 2 display the results of FQMR-QMR, Tables 3 and 4 display the results of FQMR-QMR(ILU(0)), and Tables 5 and 6 display the results of FQMR-CGNE. We list the average number of inner iterations needed to reach the inner tolerance, the exact number of outer iterations needed to reach the outer tolerance, and the number of operations used to complete the solution. In Tables 3 and 4, we point out that, for an inner tolerance of 10^{-1}, FQMR cannot achieve full accuracy in the outer iteration; thus for this case, QMR(ILU(0)) is not a good preconditioner. For these tables we list the outer tolerance separately at each step. We remark that a more efficient implementation of FQMR-QMR is possible where steps (8) and (9)

TABLE 3
FQMR-QMR(ILU(0)). $\beta = -100, \gamma = 10$.

Out. tol.	Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-4}	10^{-1}	126	31	5.96×10^{8}
10^{-7}	10^{-2}	43	36	2.31×10^{8}
10^{-7}	10^{-3}	30	38	1.74×10^{8}
10^{-7}	10^{-4}	35	40	2.09×10^{8}
10^{-7}	10^{-5}	13	37	7.28×10^{7}
10^{-7}	10^{-6}	11	39	$\mathbf{6.44\times10^{7}}$

TABLE 4
FQMR-QMR(ILU(0)). $\beta = 10, \gamma = 1000$.

Out. tol.	Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-3}	10^{-1}	64	31	3.03×10^{8}
10^{-7}	10^{-2}	8	36	4.37×10^{7}
10^{-7}	10^{-3}	3	59	2.67×10^{7}
10^{-7}	10^{-4}	2	78	$\mathbf{2.34\times10^{7}}$
10^{-7}	10^{-5}	2	103	3.08×10^{7}
10^{-7}	10^{-6}	2	123	3.70×10^{7}

TABLE 5
FQMR-CGNE. $\beta = -100, \gamma = 10$, *out. tol.* $= 10^{-7}$.

Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-1}	10	636	4.69×10^{8}
10^{-2}	10	729	5.38×10^{8}
10^{-3}	8	775	4.57×10^{8}
10^{-4}	7	729	3.77×10^{8}
10^{-5}	2	565	$\mathbf{8.35\times10^{7}}$
10^{-6}	2	669	9.89×10^{7}

TABLE 6
FQMR-CGNE. $\beta = 10, \gamma = 1000$, *out. tol.* $= 10^{-7}$.

Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-1}	15	512	5.67×10^{8}
10^{-2}	4	209	6.42×10^{7}
10^{-3}	3	289	6.21×10^{7}
10^{-4}	2	278	$\mathbf{4.02\times10^{7}}$
10^{-5}	2	423	6.26×10^{7}
10^{-6}	2	441	6.52×10^{7}

of Algorithm 2.1 are performed with a single call to QMR, but we have not used this feature here.

As it can be observed, reducing the inner tolerance produces a better preconditioner, and the overall convergence is improved. As is to be expected, the average number of inner iterations increases. An important observation comes from looking at the progression of total number of operations as the inner tolerance decreases from 10^{-1} to 10^{-6}. For our given outer tolerance of 10^{-7}, the amount of required operations in relation to the inner tolerance will decrease to a point and then begin to increase.

Table 7
FQMR-QMR: $\beta = -100, \gamma = 10$, *outer tol.*$= 10^{-4}$.

Inner tol.	Matrix dimension	Out. it.	Inner it.	Operations
10^{-1}	1024	5	96	5.63×10^{7}
10^{-1}	4096	5	187	4.38×10^{8}
10^{-1}	10000	5	276	1.58×10^{9}
10^{-1}	40000	5	1055	2.41×10^{10}
10^{-2}	1024	2	113	3.88×10^{7}
10^{-2}	4096	8	828	3.10×10^{9}
10^{-2}	10000	3	1134	3.88×10^{9}
10^{-2}	40000	3	1527	2.09×10^{10}
10^{-3}	1024	2	124	2.91×10^{7}
10^{-3}	4096	2	249	4.38×10^{8}
10^{-3}	10000	3	1181	4.05×10^{9}
10^{-3}	40000	2	2294	2.09×10^{10}

This phenomenon is consistent with the behavior of other inner-outer methods; see e.g., [5], [24]. In Tables 1, 2, 4, and 6, the smallest amount of work was achieved for an inner tolerance of 10^{-4}; in Table 5 the smallest amount of work was achieved for an inner tolerance of 10^{-5}; while in Table 3 an inner tolerance of 10^{-6} yielded the least amount of work. This demonstrates that the inner iterative method need not, in every case, be solved to the fullest precision in order to have a good preconditioner; see [4] for other examples of this occurrence. Thus, for a given flexible preconditioner and a specific outer residual norm tolerance, we can find an optimal choice of inner tolerance for minimizing work. It can be observed that this optimal choice is problem dependent. Note also that choosing an inner tolerance equal to the outer one, say, 10^{-7} in most of our cases, would imply only one outer iteration. This is equivalent to just running the inner iterative method.

We next give the results of our experiments with larger matrices A. We solve the indefinite problem, $\beta = -100, \gamma = 10$, using FQMR-QMR with varying grid sizes of 32, 64, 100, and 200, giving us matrices of dimension 1024, 4096, 10000, and 40000, respectively. Table 7 records the results for an outer tolerance of 10^{-4}. We give the results for each of the matrix sizes using the inner tolerances 10^{-1}, 10^{-2}, and 10^{-3}. We point out that for the total number of outer iterations there is little or no change. Thus, the increase in the work per variable is wholly a result of an increase in the number of inner iterations.

We present now several figures which display that in many cases the maximum attainable accuracy of FQMR is better than that of the corresponding QMR. By this we mean the smallest possible relative residual norm. Figure 1 shows the maximum attainable accuracy of FQMR-QMR(ILU(0)) and QMR(ILU(0)) for the indefinite problem, $\beta = -100$, $\gamma = 10$. Here FQMR-QMR(ILU(0)) was able to achieve a relative residual norm of 10^{-7}, while QMR(ILU(0)) terminated at 10^{-4}. This observation is typical of all our experiments with FQMR. One particularly strong example of this behavior is observed for the matrix created with $\beta = -1000.1$ and $\gamma = 10.0$. The convergence curves of QMR and FQMR-QMR for this matrix are shown in Figure 2. Notice that while QMR stagnates at 10^{-2}, we achieve a relative residual norm of 10^{-9} using FQMR-QMR for the same number of operations. FQMR-QMR can achieve an even lower relative residual norm if we allow for additional work. A value of 10^{-15} is reached in 7.42×10^{8} operations.

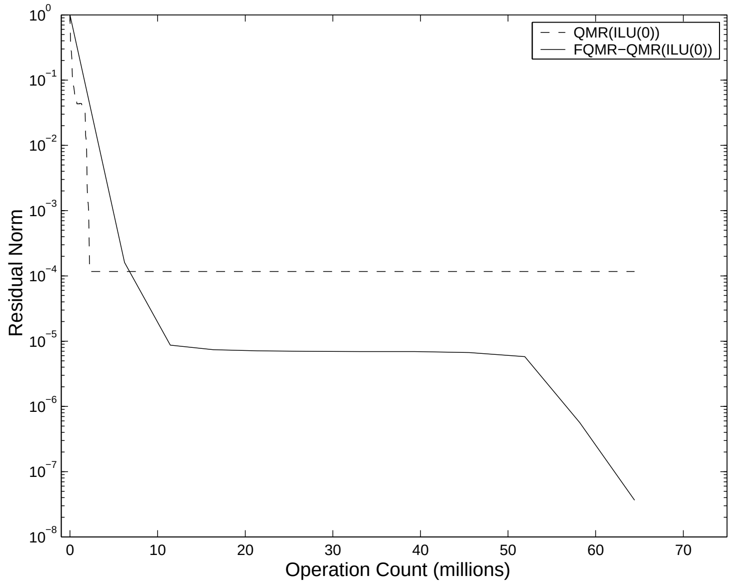

FIG. 1. *FQMR convergence:* $\beta = -100, \gamma = 10$*, inner tol.* $= 0.01$.

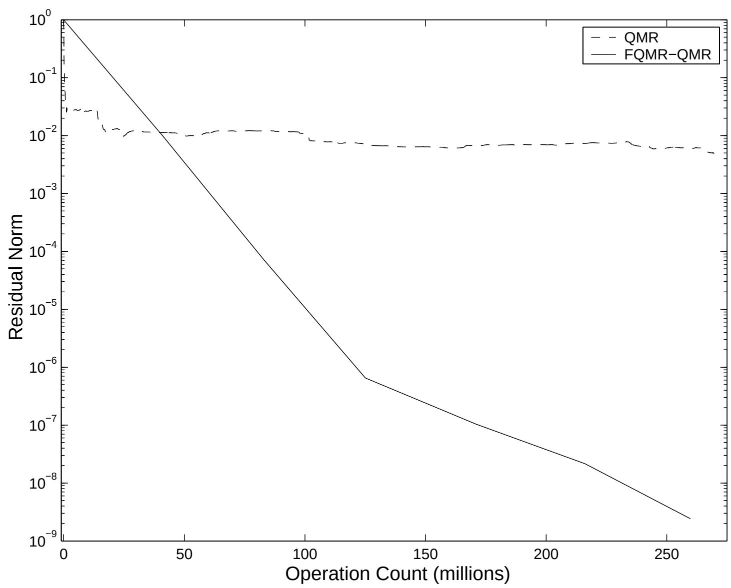

FIG. 2. *FQMR convergence:* $\beta = -1000.1, \gamma = 10$.

In Table 8, we further confirm these findings by recording achievable relative residual norms of FQMR and QMR for other choices of the matrix A. Notice that even when QMR performs well, i.e., it successfully converges to an appropriately small relative residual norm before reaching a plateau, FQMR can be shown to perform better by reaching an even smaller value. The ability to reach a lower relative residual norm by using a flexible preconditioner was observed both in the case of breakdown and stagnation. At the present time, we do not have a full explanation for this

Table 8
Comparison of achievable residual norms for FQMR-QMR and QMR.

β	γ	Res. norm - QMR	Res. norm - FQMR-QMR
-1000	10	10^{-8}	5.2×10^{-15}
1000	10	10^{-8}	6.1×10^{-15}
100	10	10^{-13}	1.42×10^{-15}
-100	10	10^{-11}	1.64×10^{-15}
10	1000	10^{-12}	5.9×10^{-15}

Table 9
*FQMR-QMR: Sherman*1 *matrix. Out. tol.* $= 10^{-7}$.

Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-1}	111	98	1.07×10^{9}
10^{-2}	10	148	1.47×10^{8}
10^{-3}	4	189	7.50×10^{7}
10^{-4}	2	180	$\mathbf{3.56\times10^{7}}$
10^{-5}	2	272	5.40×10^{7}
10^{-6}	2	327	6.28×10^{7}

phenomenon.

We comment that there are of course several ways of going beyond the point where QMR stagnates, for example, by using iterative refinement or restarting QMR. Also, if one uses the coupled two-term recurrences version of QMR, the maximum attainable residual norm is better than with the three-term recurrence version of QMR used here; see [13].

To emphasize the robustness of the new FQMR method, we ran FQMR on two matrices whose structure is different from the previous examples. These are the Sherman1 matrix and the Sherman5 matrix from [8]. They are the first and fifth matrices from the Sherman collection, respectively. Both represent oil reservoir simulations, with Sherman1 coming from a black oil simulation with shale barriers on a $10 \times 10 \times 10$ grid with one unknown per grid point, and Sherman5 coming from a fully implicit black oil simulator on a $16 \times 23 \times 3$ grid with three unknowns per grid point. The Sherman1 matrix is of dimension 1000 and has 3750 nonzeros, and the Sherman5 matrix is of dimension 3312 and has 20793 nonzeros.

Table 9 displays the convergence behavior of FQMR-QMR for the Sherman1 matrix, and Table 10 displays the convergence behavior of FQMR-QMR for the Sherman5 matrix. Notice that for both of these matrices the convergence behavior of FQMR-QMR remains comparable to what we have seen in all of the previous examples. Tables 9 and 10, also, display a consistency with our other examples in that the total work required for solving these problems with an outer tolerance of 10^{-7} reaches a minimum when the inner tolerance is 10^{-4} for Table 9 and 10^{-5} for Table 10. Thus, once more we see an optimal preconditioner for our implementation is achieved when using a less precise inner iteration.

To emphasize the property that we have observed in FQMR of achieving a lower relative residual norm than QMR, we display full convergence results of both QMR and FQMR-QMR on the Sherman5 matrix in Figure 3. Here QMR can achieve a tolerance of only 2.0×10^{-8}, while FQMR-QMR reaches 3.5×10^{-16}. Therefore, once again, FQMR can outperform QMR when an extremely low residual norm is required.

TABLE 10
FQMR-QMR: Sherman5 matrix.

Out. tol.	Inner tol.	Out. it.	Avg. inner it.	Oper.
10^{-2}	10^{-1}	15	138	8.89×10^{8}
10^{-3}	10^{-2}	2	570	4.09×10^{8}
10^{-7}	10^{-3}	16	2495	1.70×10^{10}
10^{-7}	10^{-4}	3	1475	1.90×10^{9}
10^{-7}	10^{-5}	2	1832	$\mathbf{1.57\times10^{9}}$
10^{-7}	10^{-6}	2	2069	1.77×10^{9}

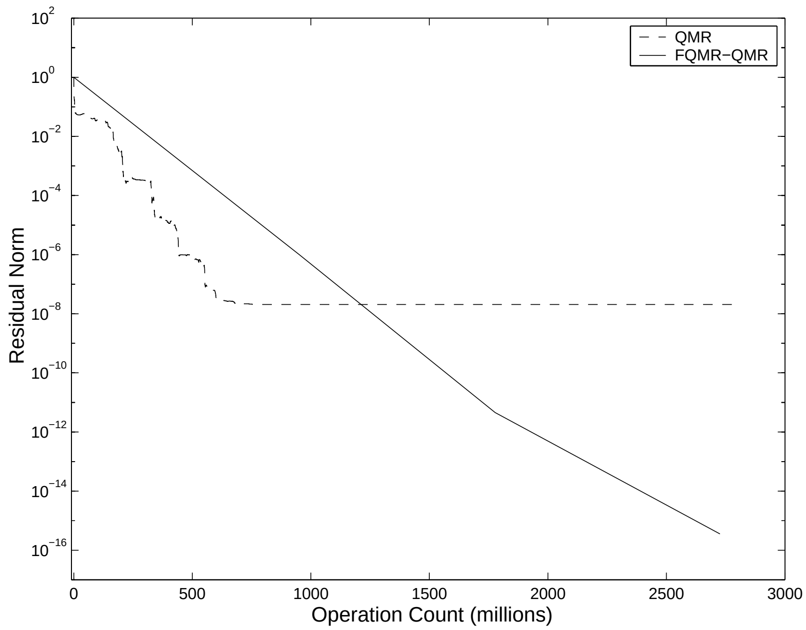

FIG. 3. *QMR vs. FQMR-QMR: Sherman5 matrix.*

6. Conclusions. We have formulated a flexible version of QMR for the solution of large sparse non-Hermitian nonsingular systems of linear equations. This new method, FQMR, converges to the solution of the linear system, as long as the new vectors generated at each step are linearly independent of the previous ones. Theoretical bounds on the norm of the residual at each step were given. These bounds are (as is to be expected) not as good as those obtained using the same preconditioner at each step. The advantage is that the variable preconditioner can be less onerous. Furthermore, there is the potential of great gains in cases of an adaptive preconditioner. One of the advantages of FQMR over FGMRES is the fact that the low memory requirements are fixed from the beginning.

Using the methodology developed to produce the mentioned bounds, we have also contributed to the analysis of FGMRES [21].

Numerical experiments of the type found in [21] illustrate the convergence behavior of FQMR and demonstrate that FQMR is capable of attaining lower residual norms than the standard QMR with three-term recurrence. Other experiments presented show a similar behavior.

Acknowledgments. We thank the referees, as well as Michele Benzi and Valeria Simoncini, for their valuable comments and suggestions. We greatly benefited from them.

REFERENCES

[1] O. Axelsson and P. S. Vassilevski, *A black box generalized conjugate gradient solver with inner iterations and variable-step preconditioning*, SIAM J. Matrix Anal. Appl., 12 (1991), pp. 625–644.

[2] J. Baglama, D. Calvetti, G. H. Golub, and L. Reichel, *Adaptively preconditioned GMRES algorithms*, SIAM J. Sci. Comput., 20 (1998), pp. 243–269.

[3] R. B. Bramley, *SPLIB Software Package*, Indiana University, Bloomington, IN, 1995.

[4] A. Bouras and V. Frayssé, *A Relaxation Strategy for Inexact Matrix-Vector Products for Krylov Methods*, Technical Report TR/PA/00/15, CERFACS, Toulouse, France, 2000.

[5] M. J. Castel, V. Migallón, and J. Penadés, *On Parallel two-stage methods for Hermitian positive definite matrices with applications to preconditioning*, Electron. Trans. Numer. Anal., 12 (2001), pp. 88–112.

[6] R. S. Dembo, S. C. Eisenstat, and T. Steihaug, *Inexact Newton methods*, SIAM J. Numer. Anal., 19 (1982), pp. 400–408.

[7] E. De Sturler, *Truncation strategies for optimal Krylov subspace methods*, SIAM J. Numer. Anal., 36 (1999), pp. 864–889.

[8] I. S. Duff, R. G. Grimes, and J. G. Lewis, *Sparse matrix test problems*, ACM Trans. Math. Software, 15 (1989), pp. 1–14.

[9] M. Eiermann and O. G. Ernst, *Geometric aspects in the theory of Krylov subspace methods*, Acta Numer., to appear.

[10] H. C. Elman, O. G. Ernst, and D. P. O'Leary, *A Multigrid Method Enhanced by Krylov Subspace Iteration for Discrete Helmholtz Equations*, Technical Report CS-TR 4029, University of Maryland, Institute for Advanced Computer Studies, College Park, MD, 1999.

[11] R. W. Freund and N. M. Nachtigal, *QMR: A quasi-minimal residual method for non-Hermitian linear systems*, Numer. Math., 60 (1991), pp. 315–339.

[12] R. W. Freund and N. M. Nachtigal, *QMRPACK Software Package*, NASA Ames Research Center, Moffet Field, CA, 1993.

[13] R. W. Freund and N. M. Nachtigal, *An implementation of the QMR method based on coupled two-term recurrences*, SIAM J. Sci. Comput., 15 (1994), pp. 313–337.

[14] A. Frommer and D. B. Szyld, *H-splittings and two-stage iterative methods*, Numer. Math., 63 (1992), pp. 345–356.

[15] G. H. Golub and M. L. Overton, *The convergence of inexact Chebyshev and Richardson iterative methods for solving linear systems*, Numer. Math., 53 (1988), pp. 571–593.

[16] G. H. Golub and Q. Ye, *Inexact preconditioned conjugate gradient method with inner-outer iteration*, SIAM J. Sci. Comput., 21 (1999), pp. 1305–1320.

[17] A. Greenbaum, *Iterative Methods for Solving Linear Systems*, Frontiers Appl. Math. 17, SIAM, Philadelphia, 1997.

[18] P. Guillaume, Y. Saad, and M. Sosonkina, *Rational Approximation Preconditioners for General Sparse Linear Systems*, Technical Report umsi-99-209, University of Minnesota, Minneapolis, 1999.

[19] N. M. Nachtigal, *A Look-Ahead Variant of the Lanczos Algorithm and Its Application to the Quasi-Minimal Residual Method for Non-Hermitian Linear Systems*, Ph.D. thesis, Massachusetts Institute of Technology, Cambridge, MA, 1991.

[20] Y. Notay, *Flexible conjugate gradient*, SIAM J. Sci. Comput., 22 (2000), pp. 1444–1460.

[21] Y. Saad, *A flexible inner-outer preconditioned GMRES algorithm*, SIAM J. Sci. Comput., 14 (1993), pp. 461–469.

[22] Y. Saad, *Iterative Methods for Sparse Linear Systems*, PWS Publishing, Boston, 1996.

[23] Y. Saad and M. H. Schultz, *GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 856–869.

[24] D. B. Szyld and M. T. Jones, *Two-stage and multisplitting methods for the parallel solution of linear systems*, SIAM J. Matrix Anal. Appl., 13 (1992), pp. 671–679.

[25] H. A. Van der Vorst and C. Vuik, *GMRESR: a family of nested GMRES methods*, Numer. Linear Algebra Appl., 1 (1994), pp. 369–386.