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SIMPLER BLOCK GMRES FOR NONSYMMETRIC SYSTEMS WITH MULTIPLE RIGHT-HAND SIDES*

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Abstract. A Simpler Block GMRES algorithm is presented, which is a block version of Walker and Zhou's Simpler GMRES. Similar to Block GMRES, the new algorithm also minimizes the residual norm in a block Krylov space at every step. Theoretical analysis shows that the matrix-valued polynomials constructed by the new algorithm is the same as the original one. However, Simpler Block GMRES avoids the factorization of a block upper Hessenberg matrix. In consequence, it is much simpler to program and requires less work. Numerical experiments are conducted to illustrate the performance of the new block algorithm.

Key words. linear systems, iterative methods, block methods, GMRES, Simpler GMRES

AMS subject classifications. 65F10

1. Introduction.

Block GMRES [13] and its variants [1, 6, 7] are effective for solving large nonsymmetric systems with multiple right-hand sides of the form

$$AX = B,$$

where A is a nonsingular matrix of order n, and $X = (x_1, \cdots, x_p)$ and $B = (b_1, \cdots, b_p)$ are rectangular matrices of dimension $n \times p$ with $p \leq n$. These block methods often promise favorable convergence properties [8, 10], and may be effectively implemented on parallel processors. In practice, if the initial block residual is nearly rank deficient, Block GMRES should be implemented with initial deflation [2].

Of interest here is the original Block GMRES. Detailed descriptions can be found in [8, 9, 11]. It is essentially identical to standard GMRES, except that operations are performed with multiple vectors instead of single vectors. Given an initial guess X_0 and $R_0 = B - AX_0$, Block GMRES generates an approximate solution X_m over the block Krylov subspace

$$K_m(A, R_0) = span(R_0, AR_0, \cdots, A^{m-1}R_0).$$

The approximate solution is of the form $X_m = X_0 + Z_m$, in which Z_m solves the minimization problem

$$\min_{Z \in K_m(A,R_0)} \|R_0 - AZ\|_F, \tag{1.1}$$

with $\|\cdot\|_F$ the Frobenius norm.

Suppose that a block orthonormal sequence $\{V_1, \cdots, V_m, V_{m+1}\}$, with each V_i being orthonormal, has been produced by the Block Arnoldi process (normally based on a Modified Block Gram-Schmidt procedure) with the initial block residual R_0. Let m be the block dimension of the basis $U_m = (V_1, \cdots, V_m)$ of $K_m(A, R_0)$. Denote by $\bar{H}_m$ the block upper Hessenberg matrix for which $AU_m = U_{m+1}\bar{H}_m$, by I_p the $p \times p$ identity matrix, and by O_p the zero matrix of order p. Furthermore, $E_i = (O_p, \cdots, I_p, \cdots, O_p)^T$ is the rectangular matrix whose ith block element is I_p, and $\bar{R}_0$ is the $p \times p$ matrix resulting from the QR factorization $R_0 = V_1\bar{R}_0$. We can write $Z_m = Z = U_mY_m$ with some $mp \times p$ matrix Y_m,

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and $R_m = R_0 - AZ_m$. Then the minimization problem (1.1) is equivalent to the block least squares problem

$$\eta_m = \min_{Y \in \mathbb{R}^{mp \times p}} \|E_1 \bar{R}_0 - \bar{H}_m Y\|_F. \tag{1.2}$$

This problem can be solved recursively for each index j up to m by updating the QR factorization of $\bar{H}_j$ $(j \leq m)$ with Givens rotations. The Frobenius norm $\eta_j = \|E_1 \bar{R}_0 - \bar{H}_j Y_j\|_F$ of the minimum residual of such a least square problem (with E_1 of size $(j+1)p \times p$ and $\bar{H}_j$ of size $(j+1)p \times jp$ now) can then be computed even before the solution $Y_j = Y$ is determined, and this norm η_j is equal to the minimum norm in (1.1). After a certain number of steps, which is normally denoted by m, the algorithm is restarted if it has not yet converged.

Summarizing we can sketch the ordinary Block GMRES algorithm with restart after m steps, and, for simplicity, based on Classical Block Gram-Schmidt, as follows.

ALGORITHM 1.1 (Block GMRES).

(i) Given X_0, set $R_0 = B - AX_0$. If $\|R_0\|_F \leq$ TOL, accept X_0 and exit; otherwise, compute a QR factorization of R_0: $R_0 = V_1 H_{11}$.

(ii) Iterate: for $j = 1, \cdots, m$, do

- *$H_{ij} = V_i^T AV_j$, $i = 1, \cdots, j$. (These are the possibly nonzero block elements of the jth block column of $\bar{H}_m$, except for the last one on the subdiagonal.)*
- *$\hat{V}_j = AV_j - \sum_{i=1}^{j} V_i H_{ij}$.*
- *Compute a QR factorization of $\hat{V}_j$: $\hat{V}_j = V_{j+1} H_{j+1,j}$.*
- *Determine the Frobenius norm η_j of the residual $E_1 \bar{R}_0 - \bar{H}_j Y_j$ of the least square problem* (1.2) with m replaced by j. (There is no need to determine the solution $Y_j = Y$ yet.)
- If $\eta_j \leq$ TOL, then go to (iv).

(iii) Set $j = m$ on exiting the loop.

(iv) Compute the solution $Y_j = Y$ of the least square problem (1.2), and form the approximate solution $X_j = X_0 + U_j Y_j$. If $\eta_j \leq$ TOL, then accept X_j and exit; otherwise, restart: set $X_0 = X_j$ and go to (i).

An essential component of Block GMRES is the Block Arnoldi process in (*ii*). It usually starts with the initial block residual R_0. By shifting the Block Arnoldi process to begin with AR_0 instead of R_0, we obtain a Simpler Block GMRES that does not require the QR factorization of a block upper Hessenberg matrix. In this case, $\{R_0, V_1, \cdots, V_{m-1}\}$ is a basis of $K_m(A, R_0)$, and (1.2) is replaced by an upper triangular least squares problem, which can be solved immediately.

In Section 2 the Simpler Block GMRES algorithm is formulated. In Section 3 an equivalence between Block and Simpler Block GMRES is established. The numerical stability of the new algorithm is also discussed. In Section 4 the two algorithms are compared by using two test matrices taken from the Matrix Market. The following notation is used. Subscripts denote the iteration index and superscripts distinguish between individual columns in a block. The symbols vec and $\otimes$ denote the vectorizing operation and the Kronecker product, respectively. The spectral 2-norm of a matrix A is denoted by $\|A\|_2$. Moreover, $\sigma_{max}(A)$ is the largest singular value of A, and $\sigma_{min}(A)$ the smallest one. The condition number of a matrix is $\kappa(A) = \sigma_{max}(A)/\sigma_{min}(A)$. $\bar{Q}_m$ and $\bar{R}_m$ are the factors of a QR factorization of R_m.

2. Simpler Block GMRES.

Suppose that R_0 is of full rank. Since A is nonsingular, AR_0 is also of full rank, and in the QR factorization $AR_0 = V_1 T_{11}$ the $p \times p$ upper triangular matrix T_{11} is nonsingular.

Let $V_1, \cdots, V_m$ be the block orthonormal vectors produced by m steps of the Block Arnoldi process. For simplicity, we assume that $K_m(A, R_0)$ has block dimension m. From the Block Arnoldi process, we have $AV_{m-1} = \sum_{k=1}^{m} T_{km} V_k$ with $p \times p$ matrices T_{km}, where T_{mm} is nonsingular. Hence,

$$K_m(A, R_0) = span(R_0, V_1, \cdots, V_{m-1}), \;\; AK_m(A, R_0) = span(V_1, \cdots, V_m).$$

With square matrices S_i of order p we can write

$$R_0 = R_m + V_1 S_1 + \cdots + V_m S_m. \tag{2.1}$$

Here we have

$$V_i^T R_m = O_p \;\; (i \le m), \tag{2.2}$$

$$R_m = R_{m-1} - V_m S_m, \tag{2.3}$$

and

$$S_m = V_m^T R_{m-1}.$$

Define $W_m = (S_1^T, \cdots, S_m^T)^T$. We can write (2.1) as

$$R_0 = R_m + U_m W_m, \tag{2.4}$$

and with

$$T_m = \begin{pmatrix} T_{11} & \cdots & T_{1m} \\ & \ddots & \vdots \\ & & T_{mm} \end{pmatrix} \in R^{mp \times mp},$$

we get

$$R_0 - AZ = R_0 - A(R_0, V_1, \cdots, V_{m-1})Y = R_m + U_m(T_m Y - W_m). \tag{2.5}$$

We want to determine $Z_m \in K_m(A, R_0)$ or its coordinates $Y_m \in \mathbb{R}^{mp \times p}$ with respect to the columns of U_m such that

$$Z_m = \arg \min_{Z \in K_m(A, R_0)} \|R_0 - AZ\|_F. \tag{2.6}$$

Equation (2.5) can be written as

$$\mathrm{vec}(R_0 - AZ) = \mathrm{vec}(R_m) + (I_p \otimes U_m)\,\mathrm{vec}(T_m Y - W_m).$$

Therefore, (2.6) is equivalent to the minimization problem,

$$\min_Y \|\mathrm{vec}(R_m) + (I_p \otimes U_m)\,\mathrm{vec}(T_m Y - W_m)\|_2. \tag{2.7}$$

Denote by $span(I_p \otimes U_m)$ the space spanned by the column vectors of $I_p \otimes U_m$. With (2.2) and (2.4), we have

$$\mathrm{vec}(R_m) \perp span(I_p \otimes U_m), \;\; \mathrm{vec}(R_m) \perp span(I_p \otimes V_m).$$

It follows that $Y_m = T_m^{-1} W_m$ solves (2.7). In consequence, $Z_m = U_m Y_m$ is determined and $R_m = R_0 - AZ_m$ is the residual.

We can write (2.3) as

$$\mathrm{vec}(R_m) = \mathrm{vec}(R_{m-1}) - (I_p \otimes V_m)\,\mathrm{vec}(S_m). \tag{2.8}$$

Observing that $\mathrm{vec}(R_m) \perp span(I_p \otimes V_m)$, we derive from (2.8) that

$$\|R_m\|_F^2 = \|\mathrm{vec}(R_m)\|_2^2 = \|\mathrm{vec}(R_{m-1})\|_2^2 - \|(I_p \otimes V_m)\,\mathrm{vec}(S_m)\|_2^2.$$

Since $I_p \otimes V_m$ is a unitary matrix, we have

$$\|R_m\|_F = (\|\mathrm{vec}(R_{m-1})\|_2^2 - \|\mathrm{vec}(S_m)\|_2^2)^{1/2},$$

or

$$\begin{aligned}\|R_m\|_F &= (\|R_{m-1}\|_F^2 - \|S_m\|_F^2)^{1/2}\\ &= \|R_{m-1}\|_F(1 - (\|S_m\|_F/\|R_{m-1}\|_F)^2)^{1/2}\\ &= \|R_{m-1}\|_F \sin(\arccos(\|S_m\|_F/\|R_{m-1}\|_F)).\end{aligned} \tag{2.9}$$

The last formula can be used to update the residual norm even if the block residual itself is not updated.

Summarizing we obtain the following Simpler Block GMRES algorithm. Again, we formulate it with restart after m steps, and, for simplicity, based on Classical Block Gram-Schmidt instead of Modified Block Gram-Schmidt in the Block Arnoldi process.

ALGORITHM 2.1 (Simpler Block GMRES).

(i) Given X_0, set $R_0 = B - AX_0$. If $\|R_0\|_F \le TOL$, accept X_0 and exit; otherwise, compute a QR factorization of AR_0: $AR_0 = V_1T_{11}$.

(ii) Iterate: for $j = 1, \cdots, m$, do
- *$T_{ij} = V_i^T AV_j, i = 1, \cdots, j-1$.*
- *$\hat{V}_j = AV_j - \sum_{i=1}^{j-1} V_iT_{ij}$ if $j > 1$.*
- *Compute a QR factorization of $\hat{V}_j$: $\hat{V}_j = V_jT_{jj}$.*
- *Either compute $S_j = V_j^T R_{j-1}$ and $R_j = R_{j-1} - V_jS_j$ or compute $\|R_j\|_F$ from the recursion (2.9).*
- *If $\|R_j\|_F \le TOL$, then go to (iv).*

(iii) Set $j = m$ on exiting the loop.

(iv) Solve the triangular system $T_jY_j = W_j$ for Y_j and form the approximate solution

$$X_j = X_0 + (R_0, V_1, \cdots, V_j)Y_j$$

If $\|R_j\|_F \le TOL$, then accept X_j and exit; otherwise, restart: set $X_0 = X_j$ and go to (i).

REMARK 2.2. To improve the numerical stability, we may use $R_0 = R_0/\|R_0\|_F$ instead of R_0 in the practical implementation. This is explained in the following section.

3. A comparison with Block GMRES. The following theorem establishes an equivalence between the matrix-valued polynomials of Block GMRES and those of Simpler Block GMRES.

THEOREM 3.1. *Suppose that m steps of Block GMRES and m steps of Simpler Block GMRES have been taken, respectively. Then, the matrix-valued polynomials constructed by the two algorithms are the same.*

Proof. Let $\Phi_m(z)$ and $\Psi_m(z)$ be the matrix-valued polynomials constructed by Block GMRES and Simpler Block GMRES, respectively. And let R_m^{BG} and R_m^{SBG} denote the residuals of the two methods. We have

$$R_m^{BG} = \Phi_m(A) \circ R_0 = R_0 - \sum_{i=0}^{m-1} A^{i+1}R_0C_i$$

and

$$R_m^{SBG} = \Psi_m(A) \circ R_0 = R_0 - \sum_{i=0}^{m-1} A^{i+1} R_0 D_i,$$

where C_i and D_i are $p \times p$ matrices, and where the notation $\circ$ is attributed to Gragg [3]. Thus,

$$R_m^{BG} - R_m^{SBG} = \sum_{i=0}^{m-1} A^{i+1} R_0 (D_i - C_i) \in AK_m(A, R_0). \tag{3.1}$$

If we let $K_m = (R_0, AR_0, \cdots, A^{m-1}R_0)$ and $F_i = D_i - C_i$, we can write (3.1) as

$$\mathrm{vec}(R_m^{BG} - R_m^{SBG}) = (I_p \otimes (AK_m))\mathrm{vec}(F) \in span(I_p \otimes (AK_m))$$

with $F = (F_0^T, \cdots, F_{m-1}^T)^T$. It is easily seen that

$$\mathrm{vec}(R_m^{BG}) \perp span(I_p \otimes (AK_m)), \;\; \mathrm{vec}(R_m^{SBG}) \perp span(I_p \otimes (AK_m)).$$

In consequence,

$$\mathrm{vec}(R_m^{BG} - R_m^{SBG}) \perp span(I_p \otimes (AK_m)).$$

We then have $\mathrm{vec}(R_m^{BG} - R_m^{SBG}) = 0$. Equivalently, $(I_p \otimes (AK_m))\mathrm{vec}(F) = 0$. Since

$$rank(I_p \otimes (AK_m)) = rank(I_p) \times rank(AK_m),$$

$I_p \otimes (AK_m)$ is of full rank. Therefore, $F = 0$ and hence $C_i = D_i$, indicating that the two matrix-valued polynomials are the same. □

Note that when $p = 1$, the theorem reduces to [5, Theorem 1].

Theorem 3.1 indicates that m steps of Simpler Block GMRES is equivalent to m steps of Block GMRES. On the other hand, because no QR factorization of a block upper Hessenberg matrix is required, the new algorithm is easier to program and requires $O(p^2m^2)$ fewer arithmetic operations than the original one. For Block GMRES, it is well known that the number of iterations for termination is expected to decrease as the number of right-hand sides increases. However, the QR factorization of a block upper Hessenberg matrix is time consuming. Thus the new algorithm offers improvements over the original one. It has been observed [4, 12], however, that Simpler GMRES is, in general, less accurate than GMRES. In fact, Simpler GMRES is inherently unstable due to the choice of the basis $\{R_0, V_1, \cdots, V_{m-1}\}$. But, in practice, Simpler GMRES works well if we do not need very high accuracy and if we restart frequently enough. This has also been observed in our experiments with Simpler Block GMRES; see Section 4.

In the following, another theorem is established. It indicates that the condition $P_m = (R_0, V_1, \cdots, V_{m-1})$ can be controlled during the iteration process of Simpler Block GMRES. Note that we use $R_0/\|R_0\|_F$ instead of R_0, and therefore

$$P_m = (R_0/\|R_0\|_F, V_1, \cdots, V_{m-1}).$$

LEMMA 3.2. *Suppose that $M = (G, E_2, \cdots, E_m)$, where G is a $mp \times p$ matrix. Then $\|M\|_2 \le (1 + \|G\|_2^2)^{1/2}$.*

Proof. Consider a unit vector $L = (L_1^T, \cdots, L_m^T)^T$, with L_i being $p \times 1$ matrices. Let

$$\bar{L} = (1 - \|L_1\|_2^2)^{-1/2}(O^T, L_2^T, \cdots, L_m^T)^T,$$

with O being a $p \times 1$ zero matrix. It is easily seen that $\bar{L}$ is also a unit vector. Therefore,

$$\|ML\|_2 = \|GL_1 + (1 - \|L_1\|_2^2)^{1/2}\bar{L}\|_2 \le \|G\|_2\|L_1\|_2 + (1 - \|L_1\|_2^2)^{1/2}\|\bar{L}\|_2.$$

It follows that $\|ML\|_2 \le (1 + \|G\|_2^2)^{1/2}$. Consequently, $\|M\|_2 \le (1 + \|G\|_2^2)^{1/2}$. □

LEMMA 3.3. *Let*

$$M_m = \begin{pmatrix} \bar{R}_{m-1}\beta^{-1} & O_p & \cdots & O_p \\ S_1\beta^{-1} & I_p & \cdots & O_p \\ \vdots & \vdots & \ddots & \vdots \\ S_{m-1}\beta^{-1} & O_p & \cdots & I_p \end{pmatrix}$$

and $P_m = (R_0/\|R_0\|_F, V_1, \cdots, V_{m-1})$*, where* $\beta = \|R_0\|_F$*. Then* $\kappa(P_m) = \kappa(M_m)$*.*

Proof. Let $R_{m-1} = \bar{Q}_{m-1}\bar{R}_{m-1}$ be a QR factorization of R_{m-1}, with $\bar{R}_{m-1}$ of order p. By (2.1), we have

$$P_m = (R_{m-1}\beta^{-1} + V_1S_1\beta^{-1} + \cdots + V_{m-1}S_{m-1}\beta^{-1}, V_1, \cdots, V_{m-1}).$$

It follows that

$$P_m = (\bar{Q}_{m-1}, V_1, \cdots, V_{m-1})M_m.$$

Since $(\bar{Q}_{m-1}, V_1, \cdots, V_{m-1})$ is unitary, $\kappa(P_m) = \kappa(M_m)$. □

THEOREM 3.4. *For* $P_m = (R_0/\|R_0\|_F, V_1, \cdots, V_{m-1})$ *and* $\|R_{m-1}\|_F \le \|R_0\|_F$*, we have* $\kappa(P_m) \le 2p^{1/2}\kappa(R_{m-1})\|R_0\|_F/\|R_{m-1}\|_F$*.*

Proof. By Lemma 3.3, we can alternatively consider the condition of M_m. Let

$$G = ((\bar{R}_{m-1}\beta^{-1})^T, (S_1\beta^{-1})^T, \cdots, (S_{m-1}\beta^{-1})^T)^T.$$

Then $M_m = (G, E_2, \cdots, E_m)$. It is easily seen that $M_m^{-1} = (\bar{G}, E_2, \cdots, E_m)$, where

$$\bar{G} = ((\beta\bar{R}_{m-1}^{-1})^T, (-S_1\bar{R}_{m-1}^{-1})^T, \cdots, (-S_{m-1}\bar{R}_{m-1}^{-1})^T)^T.$$

By Lemma 3.2, we have

$$\|M_m\|_2 \le (1 + \|G\|_2^2)^{1/2}, \tag{3.2}$$

and

$$\|M_m^{-1}\|_2 \le (1 + \|\bar{G}\|_2^2)^{1/2}. \tag{3.3}$$

Let

$$\overline{G} = \begin{pmatrix} -\bar{R}_{m-1}^{-1}\beta & & & \\ & I_p & & \\ & & \ddots & \\ & & & I_p \end{pmatrix} G(-\beta\bar{R}_{m-1}^{-1}).$$

Since $\|R_{m-1}\|_F \le \|R_0\|_F$ and $\|\bar{G}\|_2 \le \|\bar{R}_{m-1}^{-1}\|_2^2\|G\|_2\beta^2$, by (3.2) and (3.3) we have

$$\kappa(M_m) \le (1 + \|G\|_2^2)^{1/2}(1 + \beta^2\|\bar{R}_{m-1}^{-1}\|_2^2\|G\|_2^2)^{1/2} \le (1 + \|G\|_2^2)\beta\|\bar{R}_{m-1}^{-1}\|_2. \tag{3.4}$$

It follows from (2.1) that

$$R_0\beta^{-1} = \bar{Q}_{m-1}\bar{R}_{m-1}\beta^{-1} + V_1S_1\beta^{-1} + \cdots + V_{m-1}S_{m-1}\beta^{-1}.$$

Equivalently,

$$R_0\beta^{-1} = (\bar{Q}_{m-1}, V_1, \cdots, V_{m-1})G.$$

Therefore,

$$\|G\|_2 = \|R_0\|_2\beta^{-1} \le \|R_0\|_F\beta^{-1} = 1. \tag{3.5}$$

On the other hand, we also have

$$\|\bar{R}_{m-1}^{-1}\|_2 = \kappa(\bar{R}_{m-1})/\|\bar{R}_{m-1}\|_2 \le p^{1/2}\kappa(R_{m-1})/\|R_{m-1}\|_F. \tag{3.6}$$

By (3.4), (3.5) and (3.6), an upper bound for $\kappa(M_m)$ is established:

$$\kappa(M_m) \le 2p^{1/2}\kappa(R_{m-1})\|R_0\|_F/\|R_{m-1}\|_F.$$

Since $\kappa(P_m) = \kappa(M_m)$, the proof is complete. □

By Theorem 3.4, $\kappa(P_m)$ is bounded by $\kappa(R_{m-1})$ and $\|R_0\|_F/\|R_{m-1}\|_F$. We may choose a rather small m to have a small $\|R_0\|_F/\|R_{m-1}\|_F$, so that $\kappa(P_m)$ is controlled well. When $p = 1$, the bound reduces to the one presented in [12, Lemma 3.1] A detailed explanation for normalizing the initial residual can also be found in [12].

4. Numerical experiments. In this section, Simpler Block GMRES is tested and compared with Block GMRES. For convenience, the two algorithms are denoted as SBGMRES(m) and BGMRES(m), respectively. The test matrices were taken from the Matrix Market [14]. All computations were carried out using Matlab. For each example, a plot shows $\log_{10}\|R_m\|_F$ as a function of the number of iterations is presented. We take m=10 and $X_0 = 0$. The right-hand sides are chosen randomly.

EXAMPLE 4.1. The matrix is PSMIGR3, which comes from records containing counts of persons by sex and age who migrated across counties in the USA between 1965 and 1970. It is a real unsymmetric matrix of size N=3140 with 543162 nonzero entries. We have $p = 2$ right-hand sides, restart every $m = 10$ iterations, and the convergence tolerance is $TOL = 10^{-14}$. Figure 4.1 shows that the two algorithms are almost equivalent with respect to the reduction of the residual, until the residual norm comes near the convergence tolerance.

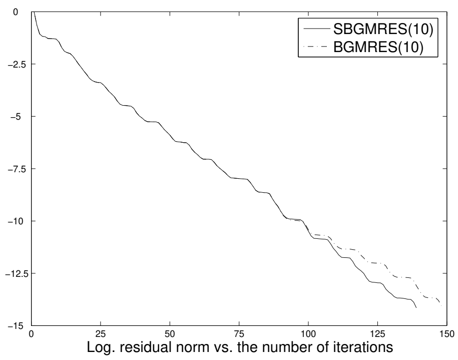

FIG. 4.1. *Example 4.1*

EXAMPLE 4.2. The matrix is JPWH991, which arises from computer random simulation of a circuit physics model. It is a real unsymmetric matrix of size N=991 with 6027 nonzero entries. We have $p = 10$ right-hand sides, restart every $m = 10$ iterations, and the convergence tolerance is $TOL = 10^{-12}$. It is seen from Figure 4.2 that SBGMRES(10) is comparable to BGMRES(10). On the other hand, recall that Simpler Block GMRES is much easier to program than Block GMRES.

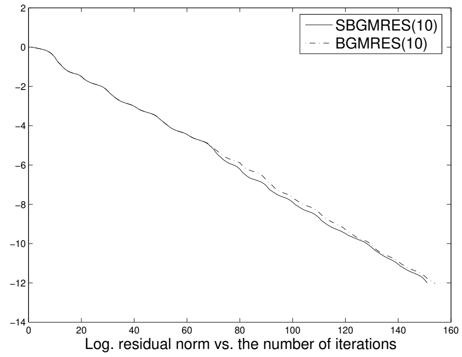

FIG. 4.2. *Example 4.2*

5. Conclusion. A Simpler Block GMRES algorithm for solving nonsymmetric systems with multiple right-hand sides was presented and studied. It was shown that m steps of Simpler Block GMRES are equivalent to m steps of Block GMRES. On the other hand, the new algorithm does not require the factorization of a block upper Hessenberg matrix, so it is easier to program and has lower computational cost per iteration. It works well in practice despite the theoretical limitations on the accuracy and conceivable problems with linear dependence of the block residuals, which, in theory, might require deflation.

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