Proceedings of ALGORITMY 2005
pp. 240–249

GMRES ACCELERATION ANALYSIS FOR A CONVECTION DIFFUSION MODEL PROBLEM*

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Abstract. When we apply the GMRES method [24] to linear systems arising from streamline upwind Petrov-Galerkin (SUPG) discretization [15, 2, 19, 9, 11] of a convection-diffusion model problem [6, 7, 8, 17, 18] on an $N \times N$ grid, convergence curves display a slow decline during initial iterations and suddenly become steeper around the Nth iteration. Whereas analysis of the initial phase of convergence was successfully accomplished, theoretical description of the second period, quantifying the observed convergence acceleration, has not been undertaken so far [18]. Exploiting tools that were used in [17, 18] to explain the period of slow convergence, we propose to analyze the phase that follows by considering a diagonal translation of the linear system. In this manner we can separate components of the system matrix that change significantly around the Nth iteration from the remaining components. We derive an upper residual bound that is based on this separation and demonstrate its accuracy on numerical examples.

Key words. Convection diffusion problem, GMRES convergence analysis, residual bound, tridiagonal non-symmetric Toeplitz matrix, diagonal translation, scaled power polynomial

AMS subject classifications. 15A09, 65F10, 65F20

1. Introduction. Partial differential equations represent problems of major importance for scientific computations. Among them, convection diffusion problems form a large class; their numerical solution has been intensively studied in the literature [19, 23, 25]. Depending on the diffusion coefficient, the differential operator can become highly non-normal [22] and the discretized operators share the non-normality. This has an influence on the choice and the behavior of solvers of the corresponding systems of linear equations. We will analyze the behavior of the frequently used GMRES method [24] when it is applied to the non-normal linear system arising from a specific convection diffusion problem with dominating convection.

Starting with an initial guess x_0, the GMRES method determines approximations x_k to the solution, with the residual vectors $r_k = b - Ax_k$ satisfying

$$\|r_k\| \,=\, \|p_k(A)r_0\| \,=\, \min_{p\in\mathcal{P}_k} \|p(A)r_0\|\,,$$

where $\mathcal{P}_k$ denotes the set of polynomials of degree at most k with value one at the origin. When the method is applied to a system that is far from normal, convergence analysis based on spectral properties of the system matrix can be very misleading [1, 9, 18, 20, 22, 13, 14]. Instead, the field of values [5, 9, 12], Faber polynomials [16], pseudospectra [22], numerical polynomial hulls [10] or simply physical observations [6] have shown to be for many non-normal discretized differential operators more reliable tools to explain the corresponding behavior of GMRES. None of these tools, however, is able to fully explain convergence behavior for the general non-normal case and such a tool is not expected to be found in the near future.

We analyze in this contribution a frequently considered model problem [9, 6, 7, 8, 11, 17, 18] with a non-normal linear system that yields distinct phases of convergence

*This work was supported by the Program Information Society under project 1ET400300415.

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of the GMRES method. We treat individual phases and analyze their behavior. In Section 2 we present the model problem, in Section 3 we analyze the initial phase of convergence with the help of tools developed by Liesen and Strakoš in [17, 18] and in the next section we show how we can extend the approach of [17, 18] in order to understand the second phase of convergence. We demonstrate the results of the analysis of the second phase with a numerical experiment in the last section, where we also briefly mention a way to describe the possible third phase of convergence.

This contribution presents in a short form some results which will be described with full proofs and analysis in [3].

2. The Model Problem. In [17, 18] Liesen and Strakoš considered, similarly to [6, 7, 8, 9, 11], the following model problem

$$-\nu\nabla^2 u + w\cdot\nabla u = 0 \quad \text{in} \quad \Omega = (0,1)\times(0,1), \quad u = g \text{ on } \partial\Omega, \tag{2.1}$$

where ν is a scalar diffusion coefficient and w is the vector velocity field. Using the SUPG discretization [15, 2, 19, 9, 11], the coefficient matrix for the discretized system takes the form

$$\tilde{A} = \nu A_d + A_c + \hat{\delta} A_s,$$

where $A_d = \langle \nabla\phi_j, \nabla\phi_i\rangle$ represents the diffusion term, $A_c = \langle w\cdot\nabla\phi_j, \phi_i\rangle$ represents the convection term, and $A_s = \langle w\cdot\nabla\phi_j, w\cdot\nabla\phi_i\rangle$ is a stabilization term added to suppress nonphysical oscillations. Here ϕ_j, $j = 1, 2, \ldots$, are the bilinear finite element nodal basis functions for an N by N grid with spacing $h = 1/(N+1)$ and $\langle\cdot,\cdot\rangle$ denotes the L^2 inner product on Ω. The parameter $\hat{\delta}$ is chosen in what has been shown to be a near optimal way for one dimensional problems and what appears to be a reasonable way for higher dimensional problems as well [6, 7], namely,

$$\hat{\delta} = \frac{\delta h}{\|w\|}, \quad \text{where} \quad \delta = \frac{1}{2}\left(1 - \frac{1}{P_h}\right),$$

and $P_h \equiv h\|w\|/(2\nu)$ is the mesh Peclet number.

For the special case of a vertical wind $w = [0,1]^T$ and the vertical line ordering (parallel with the wind direction) for equations and unknowns, the N^2 by N^2 system matrix A_V takes the form

$$A_V = A_V(h,\nu,\delta) = \nu K\otimes M + M\otimes((\nu+\delta h)K + G), \tag{2.2}$$

see, e.g., [4, Section 1.1] and [9, pp. 1081 and 1089]. Here

$$M = \frac{h}{6}(S + 4I + S^T), \tag{2.3}$$

$$K = \frac{1}{h}(-S + 2I - S^T), \tag{2.4}$$

$$G = \frac{1}{2}(-S + S^T), \tag{2.5}$$

where I is the identity and $S = [e_2, \ldots, e_N, 0]$ is the down shift matrix, are the N by N mass, stiffness and gradient matrices of the one dimensional constant coefficient convection diffusion equation discretized on a uniform mesh using linear elements. The symmetric tridiagonal Toeplitz matrices M and K can be diagonalized by the

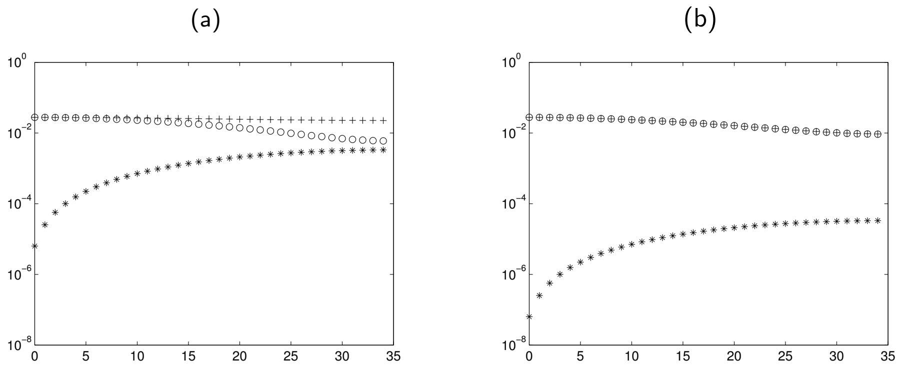

FIG. 2.1. *Entries* $|\gamma_j|$ *(o),* $|\gamma_j\tau_j|$ *(+) and* $|\gamma_j\zeta_j|$ *(*) of the blocks* T_j *from (2.7),* $j = 1,\ldots,35$. *(a)* $\nu = .005$*; (b)* $\nu = .00005$.

same matrix of eigenvectors [18]. Denoting this matrix with U we transform the system matrix A_V through

$$(U \otimes I)A_V(U \otimes I) = \nu(UKU) \otimes M + (UMU) \otimes ((\nu + \delta h)K + G) \equiv A. \tag{2.6}$$

Elementary algebra shows that A is a block-diagonal matrix consisting of N *nonsymmetric* tridiagonal Toeplitz blocks T_j, each of size N by N,

$$A = \mathrm{diag}(T_1,\ldots,T_N), \quad T_j = \gamma_j\,(S + \tau_j I + \zeta_j\,S^T), \quad j = 1,\ldots,N, \tag{2.7}$$

for more details see [6], [7] and [18].

We consider two example problems, each with $h = 1/36$, which yields system matrices of dimension 1225. In the first case $\nu = .005$ and in the second $\nu = .00005$, giving mesh Peclet numbers of 2.778 and 277.8, respectively. In Fig. 2.1 the values $|\gamma_j|$, $|\gamma_j\tau_j|$ and $|\gamma_j\zeta_j|$, $j = 1,\ldots,35$, are displayed. Fig. 2.2(a) shows the convergence of the GMRES algorithm for each problem, using a zero initial guess and a right hand side vector corresponding to the discontinuous inflow boundary conditions

$$u(x,0) = u(1,y) = 1 \quad \text{for } \frac{1}{2} \le x \le 1 \text{ and } 0 \le y < 1, \tag{2.8}$$

$$u(x,y) = 0 \qquad \text{elsewhere on } \partial\Omega, \tag{2.9}$$

see [21] and [7, 8, 9]. Both curves display a period of slow convergence followed by an acceleration of convergence speed. For a similar behavior with a different choice of parameters see [18]. In the next section we analyze the initial phase.

3. The initial phase of convergence. We will briefly present the explanation of slow initial convergence of GMRES for this model problem which was given by Liesen and Strakoš in [18]. They exploit the block-diagonal structure (2.7) of the system matrices arised from the discretization of the model problem. Partitioning the right hand side b (resulting from the discontinuous inflow boundary conditions (2.8) and (2.9)) according to the block-diagonal structure as

$$b = [b^{(1)T},\ldots,b^{(N)T}]^T, \tag{3.1}$$

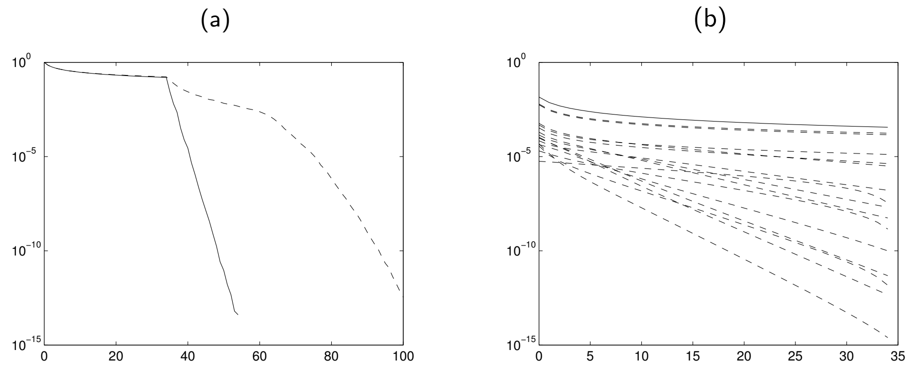

FIG. 2.2. *(a) GMRES relative residual norms for $\nu = .005$ (solid) and $\nu = .00005$ (dashed); (b) squared GMRES absolute residual norms for (2.7) with right hand side from (2.8) and (2.9) (solid) and for each system (3.4), $j = 1, \ldots, 15$, individually (dashed lines), $\nu = .005$.*

where all $b^{(j)}$ are column vectors of length N, we obtain the lower residual bound

$$\|r_k\|^2 = \min_{p \in \mathcal{P}_k} \|p(A)b\|^2 = \min_{p \in \mathcal{P}_k} \sum_{j=1}^{N} \|p(T_j)b^{(j)}\|^2 \tag{3.2}$$

$$\geq \sum_{j=1}^{N} \min_{p \in \mathcal{P}_k} \|p(T_j)b^{(j)}\|^2. \tag{3.3}$$

Hence the GMRES residual norms for the model problem are bounded from below by the residual norms generated by the individual block problems

$$T_j x^{(j)} = b^{(j)}, \qquad j = 1, 2, \ldots, N. \tag{3.4}$$

If GMRES converges slowly for at least one of the block problems, then the bound implies that GMRES must converge slowly for the *entire* problem during the first N iterations.

This is exactly what happens in our examples. In Fig. 2.2(b) the squared absolute residual norms of the slowest converging block problems (3.4) (i.e. the blocks T_1 till T_{15}) for the first problem with $\nu = 0.05$ are represented by dashed lines. The solid line displays the squared absolute residual norms for the original problem with the system matrix (2.7) and the right hand side corresponding to (2.8) and (2.9). In the second example, with $\nu = 0.0005$, the curves are very similar and we do not show them here.

Slow convergence of GMRES applied to a single block problem (3.4) with the tridiagonal Toeplitz matrix $T_j = \gamma_j\,(S + \tau_j I + \zeta_j\, S^T)$ has been analyzed in [17, 18] as follows. The analysis is based on the following identity for the kth residual vector $r_k^{(j)}$ of the jth block problem

$$\frac{(r_k^{(j)})^T}{\|r_k^{(j)}\|^2} = [1, -\tau_j, \ldots, (-\tau_j)^k][b^{(j)}, (S + \zeta_j S^T)b^{(j)}, \ldots, (S + \zeta_j S^T)^k b^{(j)}]^+\,, \tag{3.5}$$

where $[X]^+$ denotes the Moore-Penrose pseudoinverse of the matrix X and we assume that $[b^{(j)}, (S+\zeta_j S^T)b^{(j)}, \ldots, (S+\zeta_j S^T)^k b^{(j)}]$ has full column rank, see [17, equation (3.14)]. Note that the expression does not depend upon the scaling factor γ_j of the Toeplitz block. Taking norms we obtain

$$\begin{aligned} \|r_k^{(j)}\| &= \left\| [1, -\tau_j, \ldots, (-\tau_j)^k][b^{(j)}, (S+\zeta_j S^T)b^{(j)}, \ldots, (S+\zeta_j S^T)^k b^{(j)}]^+ \right\|^{-1} \\ &\geq \left(\sum_{i=0}^{k} (-\tau_j)^{2i} \right)^{-\frac{1}{2}} \sigma_{\min}\Big([b^{(j)}, (S+\zeta_j S^T)b^{(j)}, \ldots, (S+\zeta_j S^T)^k b^{(j)}] \Big) . \end{aligned} \tag{3.6}$$

In order to bound (3.6) from below, we write

$$\begin{aligned} &[b^{(j)}, (S+\zeta_j S^T)b^{(j)}, \ldots, (S+\zeta_j S^T)^k b^{(j)}] \\ &= [b^{(j)}, Sb^{(j)}, \ldots, S^k b^{(j)}] + [0, \zeta_j S^T b^{(j)}, \ldots, \left((S+\zeta_j S^T)^k - S^k\right) b^{(j)}] \\ &\equiv L_k^{(j)} + M_k^{(j)}. \end{aligned} \tag{3.7}$$

When the first entry of the right hand side $b^{(j)}$ is nonzero, the matrix $L_{N-1}^{(j)}$ is lower triangular and nonsingular. This is true for all block problems (3.4). Moreover, some of the blocks satisfy $\|M_{N-1}^{(j)}(L_{N-1}^{(j)})^{-1}\| < 1$. For these blocks and $k = N-1$ we can bound (3.6) by

$$\begin{aligned} &\left(\sum_{i=0}^{N-1} (-\tau_j)^{2i} \right)^{-\frac{1}{2}} \sigma_{\min}\Big([b^{(j)}, (S+\zeta_j S^T)b^{(j)}, \ldots, (S+\zeta_j S^T)^{N-1} b^{(j)}] \Big) \\ &\qquad \geq \Big(1 - \|M_{N-1}^{(j)}(L_{N-1}^{(j)})^{-1}\| \Big) \left(\sum_{i=0}^{N-1} (-\tau_j)^{2i} \right)^{-\frac{1}{2}} \sigma_{\min}(L_{N-1}^{(j)}) , \end{aligned} \tag{3.8}$$

see [17, 18]. Then the slow initial convergence of GMRES applied to the original $N^2 \times N^2$ problem can be quantified by the large values of the lower bound (3.8) for some dominating $N \times N$ block problems.

The main limitation of this approach lies in the fact that it treats the individual block problems separately. Although the lower bound (3.3) explains slow initial convergence, an analysis of the acceleration at step N cannot be based on (3.3) because for $k = N$ all single block problems are solved and the bound (3.3) is zero. Moreover, the phase of accelerated convergence needs to be described by an upper bound rather than a lower bound, and the upper bound should couple the influence of the single block problems on the rightmost minimization problem of (3.2).

4. Acceleration of convergence. For quantification of the acceleration of convergence we will modify the tool presented in the preceding section. Liesen and Strakoš analyze convergence by separating the influence of the diagonal from the influence of the subdiagonals, see (3.6). Having done so, they decompose the matrix related to subdiagonal entries into an easy to handle lower triangular matrix plus the remainder and concentrate on the triangular matrix, see (3.7) and (3.8). Here we will do essentially the same.

Let for some properly chosen parameter τ the matrix $C = A - \tau I$ denote a diagonal translation of $A = \mathrm{diag}(T_1, \ldots, T_N)$, $T_j = \gamma_j\,(S + \tau_j I + \zeta_j\, S^T)$, $j = 1, \ldots, N$. Then, similarly to (3.5), the GMRES residual vectors can, under the assumption that

$[b, Cb, \ldots, C^k b]$ has full column rank, be written as

$$r_k^T = \|r_k\|^2 \, [1, -\tau, \ldots, (-\tau)^k][b, Cb, \ldots, C^k b]^+,$$

for the proof see [3]. Taking norms gives

$$\|r_k\| = \left\| \left[1, -\tau, \ldots, (-\tau)^k\right] \; [b, Cb, \ldots, C^k b]^+ \right\|^{-1}. \tag{4.1}$$

Writing $C = S_L + D + S_U$, where

$$S_L = \operatorname{diag}(\gamma_1 S, \ldots, \gamma_N S), \tag{4.2}$$

$$D = \operatorname{diag}((\gamma_1 \tau_1 - \tau)I, \ldots, (\gamma_N \tau_N - \tau)I)), \tag{4.3}$$

$$S_U = \operatorname{diag}(\gamma_1 \zeta_1 S^T, \ldots, \gamma_N \zeta_N S^T), \tag{4.4}$$

we define, as in (3.7),

$$\begin{aligned} [b, Cb, \ldots, C^k b] &= [b, (S_L + D + S_U)b, \ldots, (S_L + D + S_U)^k b] \\ &= [b, S_L b, \ldots, S_L^k b] + \left[0, (D + S_U)b, \ldots, [(S_L + D + S_U)^k - S_L^k]b\right] \\ &\equiv L_k + M_k. \end{aligned} \tag{4.5}$$

With the partitioning (3.1) of b, the $(i+1)$st column of L_k has the following structure:

$$L_k e_{i+1} = S_L^i b = [(\gamma_1 S)^i b^{(1)T}, \ldots, (\gamma_N S)^i b^{(N)T}]^T.$$

Every vector $(\gamma_j S)^i b^{(j)}$ has i leading zero entries due to the application of the down shift S^i. Clearly, all the columns of L_k starting from the $(N+1)$st column, must be zero vectors. This represents the significant change at the Nth iteration which we link to the acceleration of convergence.

We now formulate an upper bound that separates quantities related to the translation τI from those related to the remainder $A - \tau I = C$. Rewrite (4.1) as

$$\|r_k\| = \frac{1}{\| \, [1, -\tau, \ldots, (-\tau)^k] \, [L_k + M_k]^+ \|}. \tag{4.6}$$

If $L_k + M_k$ has full column rank, then for any vector v of length $k+1$,

$$\begin{aligned} \left| \, [1, -\tau, \ldots, (-\tau)^k] \, v \right| &= \left| \, [1, -\tau, \ldots, (-\tau)^k] \, [L_k + M_k]^+ (L_k + M_k) \, v \right| \\ &\le \| \, [1, -\tau, \ldots, (-\tau)^k] \, [L_k + M_k]^+ \| \, \|(L_k + M_k) \, v\|, \end{aligned}$$

hence with (4.6)

$$\|r_k\| \;\le\; \|(L_k + M_k) \, v\| \, \left| \, [1, -\tau, \ldots, (-\tau)^k] \, v \right|^{-1}.$$

With the choice $v = e_{k+1}$ we can exploit the fact that the last column of L_k must vanish for $k \ge N$. The resulting upper bound is

$$\|r_k\| \;\le\; \frac{\|(L_k + M_k) e_{k+1}\|}{|\tau|^k}. \tag{4.7}$$

Note that this upper bound is nothing but the bound we obtain by replacing the residual polynomial with the scaled and translated kth power polynomial. Indeed, using (4.5),

$$\|r_k\| = \min_{\substack{p \in \mathcal{P}_k \\ p(0)=1}} \| \, p(A) b\| \le \left\| \left(\frac{A - \tau I}{-\tau} \right)^k b \right\| = \frac{\|C^k b\|}{|\tau|^k} = \frac{\|(L_k + M_k) e_{k+1}\|}{|\tau|^k}.$$

In the next section we show that this bound captures, for a proper choice of the parameter τ, the sudden decrease of the residual norm at the Nth iteration.

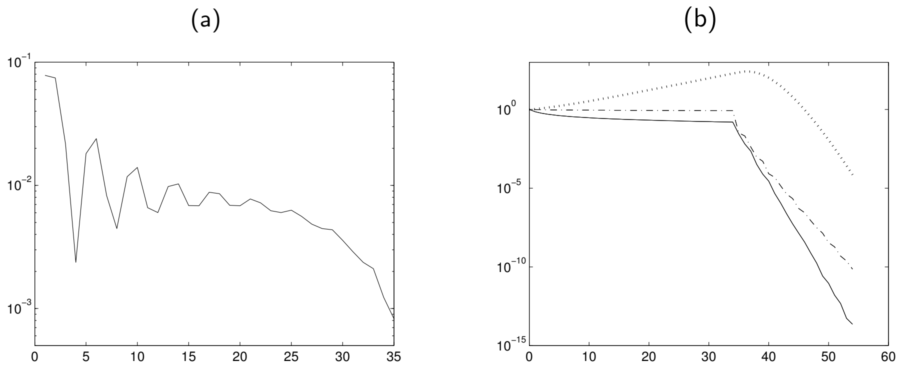

FIG. 5.1. *(a) Norms of $b^{(j)}$, $j = 1, \ldots, N$, for $\nu = .005$ (solid); (b) GMRES residual norm reduction for $\nu = .005$ (solid) and the corresponding upper bounds from (4.7) with $\tau = (\sum_{j=1}^{N} \gamma_j \tau_j)/N$ (dotted) and $\tau = (\gamma_1\tau_1 + \gamma_2\tau_2)/2$ (dash-dotted).*

5. Numerical experiment. We consider the model problem from Section 2 with the specification of boundary conditions and parameters as in Fig. 2.2(a). We concentrate in this section on the choice of the translation parameter τ, and try to obtain a bound (4.7) that captures the change of convergence behavior and that is as tight as possible. Please note from the preceding section that the more the parameter τ reduces the influence of the matrix M_k in (4.5), the better is the chance that the corresponding bounds will describe the acceleration of convergence. We will propose several choices of the translation parameter τ, compute the resulting bounds (4.7) and discuss their behavior.

Let us start with the case $\nu = .005$ (the solid curve in Fig. 2.2(a)). Then the values $\gamma_j\tau_j$, $j = 1, \ldots, 35$, are remarkably close to each other, see Fig. 2.1(a). Moreover, the norms of the vectors $b^{(j)}$ (see the solid line in Fig. 5.1(a)) show that $b^{(1)}$ and $b^{(2)}$ are much larger in norm than the others.

Based on these observations, we concentrate on the contribution from the first and the second block from (2.7), which dominate the initial stage of the minimization problem (3.2), and take $\tau \equiv \frac{(\gamma_1\tau_1+\gamma_2\tau_2)}{2}$. Then (4.7) gives the upper bound represented by the dash-dotted curve in Figure 5.1(b). It captures very tightly the slow initial decrease of the residual norm as well as the sudden acceleration of convergence. However, after a few more steps, the slope of the upper bound does not fit due to the differences between T_1, T_2 and T_j, $3 \le j \le N$, which will show up after the influence of the dominant blocks T_1 and T_2 is eliminated.

In order to get a bound that is less sensible to the differences in T_j, $1 \le j \le N$, we may try the average diagonal value, $\tau \equiv (\sum_{j=1}^{N} \gamma_j\tau_j)/N$. The resulting bound is plotted as the dotted curve in Figure 5.1(b). It does not capture the sudden change of convergence but the slope of the accelerated convergence is almost correct (though the bound is not tight).

Both choices of τ make the entries of the matrix D in (4.3) tiny. Hence, as $|\gamma_j\zeta_j|$ is much smaller than one for $j = 1, \ldots, N$, the matrix L_k is for $k = 1, \ldots, N$ much larger in norm than M_k. Therefore the corresponding bounds start to decrease significantly around the Nth step when the newly formed columns of L_k are zero. The choice $\tau = \frac{(\gamma_1\tau_1+\gamma_2\tau_2)}{2}$ yields a tighter bound because it concentrates on the blocks $T_1 - \tau I$ and $T_2 - \tau I$ corresponding to the dominating entries $b^{(1)}$ and $b^{(2)}$ of the initial residual.

With the smaller scalar diffusion parameter $\nu = .00005$, the acceleration of convergence around the 35th iteration is less pronounced than with $\nu = .005$, but it is still present (see the dashed curve in Figure 2.2(a)). We observe a slight acceleration at step 35, and a second, more significant acceleration later. The individual diagonal values $\gamma_j\tau_j$ are not as close to each other as for $\nu = .005$ (see Fig. 2.1(b)). On the other hand, the elements of b with largest absolute value are again found in $b^{(1)}$ and $b^{(2)}$, see the solid line in Fig. 5.2(a).

If we choose, as before, $\tau \equiv (\gamma_1\tau_1 + \gamma_2\tau_2)/2$, we obtain the upper bound plotted with a dash-dotted line in Figure 5.2(b) . The bound captures well the first acceleration but not the second one. This observation is explained by the construction of the bound.

In the remainder of this section we outline the construction of an upper bound which captures the slope of the third phase of convergence for $\nu = .00005$. It is based on modification of (4.7).

In the first 60 steps, the dominance of the first two residual blocks $r_0^{(1)}$, $r_0^{(2)}$ is largely reduced, as shown in Fig. 5.2(a), which plots the values of $\|r_{60}^{(j)}\|$, $j = 1, \ldots, N$, (dashed line), where we have partitioned residual vectors according to (3.1). From the 60th iteration on, we therefore change the translation parameter and use the average diagonal value $\tau \equiv (\sum_{j=21}^{35} \gamma_j\tau_j)/15$ of the 15 last blocks. This choice is motivated by the size of the individual blocks $r_{60}^{(j)}$. Thus we extend our upper bound as

$$\|r_k\| \leq \left\| \left(\frac{2A - (\gamma_1\tau_1 + \gamma_2\tau_2)I}{-(\gamma_1\tau_1 + \gamma_2\tau_2)} \right)^k r_0 \right\|, \tag{5.1}$$

for $k \leq 60$, and

$$\|r_k\| \leq \left\| \left(\frac{15A - (\sum_{j=21}^{35} \gamma_j\tau_j)I}{-(\sum_{j=21}^{35} \gamma_j\tau_j)} \right)^{k-60} \cdot \left(\frac{2A - (\gamma_1\tau_1 + \gamma_2\tau_2)I}{-(\gamma_1\tau_1 + \gamma_2\tau_2)} \right)^{60} r_0 \right\|, \tag{5.2}$$

for $k > 60$. The resulting upper bound is represented by the dashed line in Fig. 5.2(b). It captures the slope of the accelerated convergence (though with delay).

Acknowledgment. The author is very grateful for impulses for this work and many suggestions concerning formulation of Zdeněk Strakoš.

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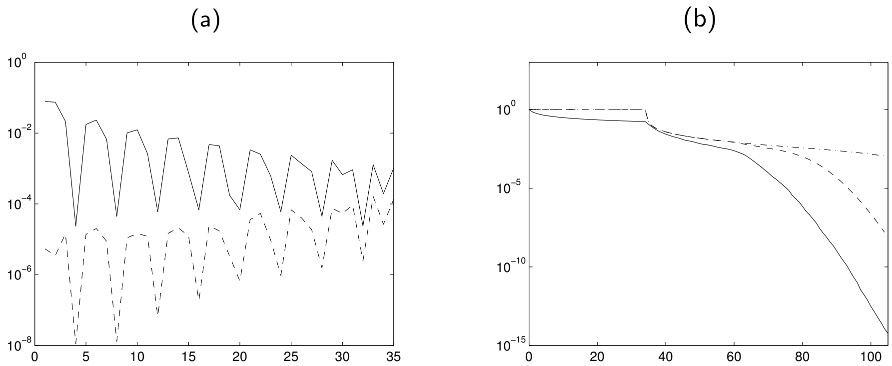

FIG. 5.2. *(a) Norms of $b^{(j)}$ (solid) and of ${r_{60}}^{(j)}$ (dashed), $j = 1, \ldots, N$, for $\nu = .00005$; (b) GMRES residual norm reduction for $\nu = .00005$ (solid); the corresponding upper bound from (4.7) with $\tau = (\gamma_1\tau_1 + \gamma_2\tau_2)/2$ (dash-dotted) and the extended bound described by (5.1) and (5.2) (dashed).*

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