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On the Performance of Various Adaptive Preconditioned GMRES Strategies

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This paper compares the performance on linear systems of equations of three similar adaptive accelerating strategies for restarted GMRES. The underlying idea is to adaptively use spectral information gathered from the Arnoldi process. The first strategy retains approximations to some eigenvectors from the previous restart and adds them to the Krylov subspace. The second strategy also uses approximated eigenvectors to define a preconditioner at each restart. This paper designs a third new strategy which combines elements of both previous approaches. Numerical results show that this new method is both more efficient and more robust.

KEY WORDS GMRES; preconditioning; invariant subspace; deflation

1. Introduction

The GMRES algorithm [16] is now a standard iterative method for solving large sparse non-symmetric linear systems of equations

$$Ax = b, \quad x \in \mathbb{R}^n \tag{1.1}$$

It uses an Arnoldi algorithm to build an orthonormal basis for Krylov subspace given by

$$K_m(A, r) = \text{Span}\{r, Ar, \ldots, A^{m-1}r\}$$

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in which an approximation to the solution of (1.1) lies. Clearly, if exact arithmetic is used, then the GMRES algorithm will converge in at most n iterations. Since the GMRES algorithm is expensive both computationally and in its memory requirements, a restarted version (GMRES(m)) is often used, in which the Krylov subspace is restricted to be of fixed dimension m and the Arnoldi process is restarted using the last iterate x_m as a new initial approximation for the restart. Unfortunately, it can be very difficult to know how to choose m a priori and if too small a value is chosen, convergence may stall.

It is known that small eigenvalues of A can slow down convergence. More recent work on the convergence behaviour of GMRES [22] relates the superlinear convergence to the convergence of Ritz values. Basically, convergence occurs as if at each iteration of GMRES the next smallest eigenvalue in magnitude is removed from the system. This work has some relation to that in [17] and [3], which show that standard stationary iteration schemes, such as Jacobi and SOR, can be rapidly accelerated by a deflation process in which the largest eigenvalues in magnitude of the amplification matrix (estimated by the power method) are periodically removed into a coupled stiff subspace (where the small stiff component is solved for by a direct method). This leads to a coupled iteration between the non-stiff and stiff subspace—the effect of which is that the fixed-point iterative scheme is rapidly accelerated.

Unfortunately, if a restarted GMRES procedure is used, the information about the smallest eigenvalues and corresponding eigenvectors is lost at each restart and so the superlinear convergence may be lost. For this reason, recently, researchers have examined different ways of reducing the negative effects of a restart.

There are several ways that this can be done, see, for example, [15] : a block-GMRES approach as in [19], an eigenvalue translation-based preconditioner [9], an augmented subspace approach [12,5] and an approximate invariant subspace-based preconditioner [7,1].

The approach based on eigenvalue translation defines a preconditioner of the form $A(I + u_1 v_1^{\mathrm{T}}) \ldots (I + u_l v_l^{\mathrm{T}})$ where the vectors $u_1, \ldots, u_l$ and $v_1, \ldots, v_l$ are chosen to condense the eigenvalues near one.

The augmented subspace solution retains vectors from the previous restart and adds them to the new subspace. In particular, it investigates saving k approximate eigenvectors of A corresponding to the k smallest eigenvalues in magnitude. These eigenvectors are estimated using a Rayleigh–Ritz method. It should be noted here that after each restart the k eigenvectors become progressively more accurate.

The method tested in [7] and [1] is to adaptively build a preconditioner for GMRES based on spectral information gathered from the Arnoldi process during iteration by restarted GMRES. The nice feature of this approach is that the advantages of preconditioning are retained without the difficulty of knowing what type of preconditioner to use. In the case of [7], after each restart the preconditioner is updated by extracting new eigenvalues corresponding to the remaining smallest eigenvalues which are smallest in magnitude. This is different from the flexible GMRES method [14] because it executes a true GMRES cycle with a constant preconditioner inside the cycle. The preconditioner is equal to the projected matrix onto the approximated invariant subspace (up to a scaling factor) and is taken as the identity on the orthogonal subspace.

Note that the preconditioner can be used on the left or the right with equal facility. The approach in [1] has a similar thrust to that in [7] and the same convergence results hold. Here they precondition on the left and the implementation uses the recurrence formulas of the Implicitly Restarted Arnoldi method defined in [20] and [11] which implies that the application of a preconditioner does not require additional evaluation of any matrix–vector

products. These recurrence formulas are truncated versions of the recurrence formulas for the QR algorithm with explicit shifts. This preconditioner is built at each restart and is applied to all the other preconditioners to give a composition effect.

The numerical results in these papers show the efficacy of these methods compared with standard restarted GMRES. However, there are still difficulties in knowing how to choose k and how many eigenvalues should be deflated at each restart. This paper addresses these issues and attempts to develop a method which combines elements of the augmented subspace solution and the automatic preconditioning approach. Thus, in Section 2 both methods are described while in Section 3 a new method combining elements of both is developed. Finally, in Section 4, numerical results are presented on five test problems: two of which come from specific real-world applications while the other three problems test the efficacy of deflation in terms of eigenvalue distribution and the conditioning of the eigenvectors. The paper concludes with a summary of the work presented and future directions.

2. Deflated GMRES

2.1. *Restarted GMRES*(m)

Let x_0 an intial guess and $r_0 = b - A * x_0$ with $\beta = \|r_0\|$. Let V_m be an orthonormal basis of the Krylov subspace $K_m(A, r_0)$ such that

$$AV_m = V_{m+1}\overline{H}_m \tag{2.1}$$

with $\overline{H}_m$ a Hessenberg matrix of order $(m + 1) \times m$. Algorithm GMRES(m) computes $x_m = x_0 + V_m y_m$ such that

$$\|b - Ax_m\| \quad = \quad \min_{y \in \mathbb{R}^m} \|\beta e_1 - \overline{H}_m y\| \tag{2.2}$$

It is known that the convergence of GMRES is similar to conjugate gradients for nearly normal systems in that small eigenvalues of A can slow convergence, but for highly non-normal systems the convergence behaviour is more complicated.

In the sequel, we assume that all eigenvalues of A are non-defective, or, in other words, that A is diagonalizable. Let $|\lambda_1| \leq |\lambda_2| \leq \ldots \leq |\lambda_n|$ be the eigenvalues of A. The following result is well known (see, for example, [6], Theorem 3.3) but we give it here along with a proof because it will help to prove the new results about our deflation methods.

Proposition 2.1. *If*

$$A = Z\Omega Z^{-1} \tag{2.3}$$

with $\Omega = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ *then after a cycle of GMRES(m)*

$$\|r_m\| \leq \|r_0\| \mathrm{cond}(Z) \min_{q \in \Pi_m^0} \max_{1 \leq i \leq n} |q(\lambda_i)|, \quad r_m = b - Ax_m \tag{2.4}$$

where Π_m^0 *is the set of polynomials* q *of degree at most* m *with* $q(0) = 1$ *and* $\mathrm{cond}(Z) = \|Z\|\|Z^{-1}\|$.

Proof
Let $r_0 = \sum_{i=1}^{n} \beta_i z_i = Z\beta$. Then $r_m = q(A)r_0$ with $q \in \Pi_m^0$ so that

$$r_m = \sum_{i=1}^{n} \beta_i q(\lambda_i) z_i \, . \tag{2.5}$$

It follows that $\|r_m\| \leq \|\beta\| \, \|Z\| \, \max_{1 \leq i \leq n} |q(\lambda_i)|$, with $\beta = (\beta_i), i = 1, \ldots, n$, but $r_0 = Z\beta$ implies $\beta = Z^{-1} r_0$ and $\|\beta\| \leq \|Z^{-1}\| \, \|r_0\|$. ■

This result, as well as various experiments, show that the smallest eigenvalues slow down the convergence. As noted in the introduction, superlinear convergence is lost when restarting GMRES(m) because the Ritz values are lost. On the other hand, the Arnoldi process can be used to compute Ritz values and Ritz vectors and to estimate eigenvalues and eigenvectors of A.

The idea underlying deflation methods is to annihilate the components of the residual r_m on the eigenvectors z_i corresponding to the smallest eigenvalues. The method to achieve this goal is to estimate these eigenvectors at each restart and to use them at the next restart. The solution developed in [12] is to augment the Krylov subspace with these estimated eigenvectors whereas the solution chosen in [7] and [1] is to define a preconditioner. In the first solution, the components of the residual are killed at the end of the cycle while the preconditioner will kill them at each internal iteration.

2.2. Adding eigenvectors

We now describe the augmented subspace method due to [12] and experimented in [5]. The method will be denoted MORGAN(m,k), where m will be the dimension of the Krylov subspace and k the maximal dimension of the invariant subspace so that the solution will be approximated in an augmented subspace of dimension $m + l$ with $l \leq k$. Let V_m be an orthonormal basis of $K_m(A, r_0)$, U a basis of the approximated invariant subspace and $W = (V_m, U)$ the basis of the augmented subspace. GMRES requires an orthogonalization of AW, which is obtained through a modified-Gram–Schmidt algorithm, so that

$$AW = V\overline{H} \tag{2.6}$$

where $V = (V_{m+1}, V_l)$ is orthogonal of size $n \times (m + 1 + l)$ and H is a Hessenberg matrix of size $(m + 1 + l) \times (m + l)$.

Algorithm MORGAN(m,k) computes $x_m = x_0 + Wy_m$ such that

$$\|b - Ax_m\| \quad = \quad \min_{y \in \mathbb{R}^{m+l}} \|\beta e_1 - \overline{H} y\| \, . \tag{2.7}$$

Algorithm: MORGAN(m,k)

ϵ is the tolerance for the residual norm;
convergence:= false;
choose x_0;
$U := \{\}$;
$l := 0$;
until convergence **do**

$r_0 = b - Ax_0$;
Arnoldi process applied to A to compute V_m;
$W = (V_m, U)$;
compute AU;
orthogonalize AW to get V;
$y_m = \text{argmin}_{y \in \mathbb{R}^{m+l}} \|\beta e_1 - \overline{H} y\|$;
$x_m := x_0 + W y_m$;
if $\|b - Ax_m\| < \epsilon$ convergence := true;
else
$x_0 = x_m$;
choose $l \leq k$;
estimate l eigenvectors U of A;
endif
enddo

The choice of l and the computation of U are described later.

2.3. *Preconditioning*

We now describe the preconditioning approach due to [7] which is also developed in a slightly different way in [1]. Now M will denote a preconditioning matrix which will be updated at each restart and V_m is an orthonormal basis of the Krylov subspace $K_m(r_0, AM^{-1})$. We give here a general form of the algorithm, denoted DEFLATED-GMRES(m,k). At each restart, the algorithm applies GMRES(m) to the matrix AM^{-1}, so that

$$AM^{-1}V_m = V_{m+1}\overline{H}_m \tag{2.8}$$

where $\overline{H}_m$ is a Hessenberg matrix of size $(m+1) \times m$.

Algorithm DEFLATED-GMRES(m,k) computes $x_m = x_0 + M^{-1}V_m y_m$ such that

$$\|b - Ax_m\| \quad = \quad \min_{y \in \mathbb{R}^m} \|\beta e_1 - \overline{H}_m y\|. \tag{2.9}$$

The preconditioner M^{-1} is defined by

$$M^{-1} := I_n + U(|\lambda_n| T^{-1} - I_l)U^{\mathrm{T}} \tag{2.10}$$

where U is a set of $l \leq k$ orthonormal vectors and $T = U^{\mathrm{T}}AU$. In practice, U will span an approximate invariant subspace.

Algorithm: DEFLATED-GMRES(m,k)

ϵ is the tolerance for the residual norm;
convergence:= false;
choose x_0;
$M := I_n$;
$U := \{\}$;
$l := 0$;
until convergence **do**

$r_0 = b - Ax_0$;
Arnoldi process applied to AM^{-1} to compute V_m;
$y_m = \text{argmin}_{y \in \mathbb{R}^m} \|\beta e_1 - \overline{H}_m y\|$;
$x_m := x_0 + M^{-1} V_m y_m$;
if $\|b - Ax_m\| < \epsilon$ convergence := true;
else
$x_0 = x_m$;
choose $l \leq k$;
compute U to estimate an invariant subspace of A of size l;
compute $T := U^{\mathrm{T}} AU$;
$M^{-1} := I_n + U(|\lambda_n| T^{-1} - I_l) U^{\mathrm{T}}$;
endif
enddo

2.4. Estimating eigenvectors

Now we deal with the estimation of U, assuming l has been chosen. A first solution to estimate eigenvectors, used in [7], is to solve the oblique problem

$$V_m^*(AM^{-1} - \theta I)V_m u = 0$$

which reduces to the ordinary eigenvalue problem

$$H_m u = \theta u, \quad U = V_m u \tag{2.11}$$

where H_m is the Hessenberg matrix obtained from $\overline{H}_m$ by removing the last row. The classical QR algorithm for Hessenberg matrices, implemented, for example, in the LAPACK library, computes all the eigenvalues and eigenvectors which are then sorted to keep the l smallest. Some precaution is required to keep together complex conjugate eigenvalues.

A second solution, which is used in the augmented subspace approach [12,5], is to solve the harmonic problem

$$(AW)^*(A - \theta I)Wu = 0$$

which reduces to the generalized eigenvalue problem

$$Ru = \theta[QV^*W]u, \quad U = Wu, \tag{2.12}$$

with $Q\overline{H} = \begin{pmatrix} R \\ 0 \end{pmatrix}$ where Q is a unitary matrix of dimension $(m+1+l) \times (m+1)$ and R is an upper triangular matrix of order $m+l$ and $[QV^*W]$ is the matrix of order $m+l$ composed of the first $m+l$ rows of QV^*W. Here too, the generalized eigenproblem is solved by a classical procedure, as implemented in the Lapack library, and the eigenvectors are sorted with attention paid to complex conjugate eigenvalues.

In [5], it is found that the harmonic projection is more accurate than the oblique or the orthogonal projections. This harmonic projection can also be used for the preconditioning approach, as will be seen in Section 3.

A third solution, as used in [1], is to estimate eigenvectors by the Implicitly Restarted Arnoldi method, but this will not be studied here.

Now, various strategies have been implemented to choose the number l of estimated eigenvectors. In all cases, m and k are chosen in advance. In [12] and [5], $l = k$ at each restart. In [7], l increases from 0 to k with 'freq' vectors added at each restart. The same strategy occurs in [1], but only when the vectors are accurate enough.

2.5. Theoretical convergence

Both augmented subspace and preconditioned GMRES aim at annihilating the components of the residual r_m in the eigenvectors corresponding to the smallest eigenvalues. In this part, we assume that the invariant subspace span(U) is exact.

Let $Z_1 = (z_1, z_2, \ldots, z_k)$ and $Z_2 = (z_{k+1}, z_{k+2}, \ldots, z_n)$ be the eigenvectors of A corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_n$ ordered by $|\lambda_1| \leq \ldots \leq |\lambda_n|$.

The augmented subspace approach leads to the following result, which generalizes the result stated in [12].

Proposition 2.2. *Let $U = Z_1$. The residual r_m computed with MORGAN(m,k) (and l=k) satisfies*

$$\|r_m\| \leq \|r_{0,2}\| \min_{q \in \Pi_m^0} \max_{k+1 \leq i \leq n} |q(\lambda_i)| \text{cond}(Z_2) \tag{2.13}$$

where $r_0 = \sum_{i=1}^{n} \beta_i z_i$, $r_{0,2} = \sum_{i=k+1}^{n} \beta_i z_i$ and cond$(Z_2) = \|Z_2\| \|(Z_2^* Z_2)^{-1} Z_2^*\|$.

Proof
For MORGAN(m,k) we get, as shown in [12],

$$r_m = \sum_{i=k+1}^{n} \beta_i q(\lambda_i) z_i$$

so that

$$\|r_m\| \leq \|\beta_2\| \|Z_2\| \max_{k+1 \leq i \leq n} |q(\lambda_i)|$$

with $\beta_2 = (\beta_i), i = k+1, \ldots, n$. Now, since $r_{0,2} = Z_2 \beta_2$, it follows that $\beta_2 = (Z_2^* Z_2)^{-1} Z_2^* r_{0,2}$ and $\|\beta_2\| \leq \|(Z_2^* Z_2)^{-1} Z_2^*\| \|r_{0,2}\|$ and the proof is complete. ■

The preconditioning approach leads to the following result, which generalizes the result stated in [1].

Proposition 2.3. *Let U an orthonormal basis of* span(Z_1) *and M defined by (2.10). Then eigenvalues of AM^{-1} are $|\lambda_n|$ with multiplicity k and $\lambda_{k+1}, \ldots, \lambda_n$ and* span$(U) =$ span(Z_1) *is an invariant subspace of AM^{-1} corresponding to the eigenvalue $|\lambda_n|$. Let $Y_2 = (y_{k+1}, y_{k+2}, \ldots, y_n)$ be the eigenvectors of AM^{-1} corresponding to the eigenvalues $\lambda_{k+1}, \ldots, \lambda_n$. The residual r_m computed in one cycle of DEFLATED-GMRES(m,k) using M satisfies*

$$\|r_m\| \leq \min_{q \in \Pi_m^0} (q(|\lambda_n|) \|r_{0,1}\| + \max_{k+1 \leq i \leq n} |q(\lambda_i)| \, \|r_{0,2}\| \, \text{cond}(Y_2)) \tag{2.14}$$

where $r_0 = r_{0,1} + r_{0,2}$ *with* $r_{0,1} = \sum_{i=1}^{k} \beta_i z_i$, $r_{0,2} = \sum_{i=k+1}^{n} \beta_i y_i$
and $\mathrm{cond}(Y_2) = \|Y_2\| \|(Y_2^* Y_2)^{-1} Y_2^*\|$.

Proof
As far as eigenvalues are concerned, we first recall here the proof found in [7] and also in [1]. Let (U, X) be an orthonormal basis of n. In this basis, A is similar to a matrix

$$\tilde{A} = \begin{pmatrix} T & \tilde{A}_{12} \\ 0 & \tilde{A}_{22} \end{pmatrix} \tag{2.15}$$

where $T = U^{\mathrm{T}} A U$ and M^{-1} is similar to a matrix

$$\tilde{M}^{-1} = \begin{pmatrix} |\lambda_n| T^{-1} & 0 \\ 0 & I_{n-k} \end{pmatrix}. \tag{2.16}$$

The preconditioned matrix AM^{-1} is therefore similar in the basis (U, X) to the matrix

$$\tilde{A}\tilde{M}^{-1} = \begin{pmatrix} |\lambda_n| I_k & \tilde{A}_{12} \\ 0 & \tilde{A}_{22} \end{pmatrix}$$

so that its eigenvalues are $|\lambda_n|$ and the eigenvalues of $\tilde{A}_{22}$, in other words $\lambda_{k+1}, \ldots, \lambda_n$.

Since the projection of AM^{-1} onto $\mathrm{span}(U)$ is $|\lambda_n| I_k$, the vectors Z_1 are eigenvectors of AM^{-1}.

After one cycle of DEFLATED-GMRES(m,k) we get

$$r_m = q(AM^{-1}) r_0$$

The eigenvalues of AM^{-1} are $|\lambda_n|$ with multiplicity k and $\lambda_{k+1}, \ldots, \lambda_n$. Hence we get

$$r_m = q(|\lambda_n|) \sum_{i=1}^{k} \beta_i z_i + \sum_{i=k+1}^{n} \beta_i q(\lambda_i) y_i$$

so that

$$\|r_m\| \leq q(|\lambda_n|) \|r_{0,1}\| + \|\beta_2\| \|Y_2\| \max_{k+1 \leq i \leq n} |q(\lambda_i)|$$

The result follows using the same proof as before. ∎

The main difference between these convergence results is the factor $\mathrm{cond}(Z_2)$ versus the factor $\mathrm{cond}(Y_2)$. It is not clear how to relate or to compare these two quantities. These results assume that the invariant subspace $\mathrm{span}(U)$ is exact. However, an approximate set of eigenvectors can still have a beneficial effect on convergence. The formula (2.13) can be modified for approximate eigenvectors by the addition of a second term to the right-hand side [12]. Experimental convergence results will depend more on the way the eigenvectors are estimated than on the strategy to choose $l \leq k$.

As in [1], this analysis ignores the effect of pseudo-pspectra on the convergence [13]. Clearly, this preconditioner will be particularly effective if there is a cluster of eigenvalues that have a large deleterious influence on convergence.

2.6. Memory requirements and complexity

Now let us examine memory requirements and arithmetic complexity. Both methods have the same memory requirements, which are at least $(m+1+k)$ vectors and preferably $(m+1+2k)$ vectors to compare with $(m+1)$ vectors for restarted GMRES(m). Indeed, MORGAN(m,k) requires the storage of W and preferably V_k while DEFLATED-GMRES(m,k) requires storage of V_{m+1},U and preferably AU.

Both methods also have roughly the same arithmetic complexity. Indeed, the bulk is an Arnoldi process, completed either by an orthogonalization of l vectors against m other vectors or by a preconditioning which amounts to m orthogonalizations of a vector against l vectors. Also, both methods require estimations of l eigenvectors U and computation of AU.

3. New deflation method

In [5], it appears to be more accurate to estimate eigenvectors by an harmonic projection than by an oblique projection. Therefore, we implemented this method in our preconditioning deflation. The previous code, as experimented in [7], is called DEFLGMRES(m,k) and the resulting code here with an harmonic projection is called HARMONIC(m,k).

We thus solve the problem

$$(AM^{-1}V_m)^*(A-\theta I)M^{-1}V_m u = 0$$

which reduces to a similar generalized eigenvalue problem

$$R_m u = \theta[Q_m V_{m+1}^* M^{-1} V_m]u, \quad U = M^{-1}V_m u \tag{3.1}$$

with $Q_m \overline{H} = \begin{pmatrix} R_m \\ 0 \end{pmatrix}$, where Q_m is a unitary matrix of dimension $(m+1)\times(m+1)$ and R_m is an upper triangular matrix of order m.

Numerical experiments show a significant improvement of HARMONIC(m,k) over DEFLGMRES(m,k). However, for some test cases, MORGAN(m,k) performs much better. This is due to the fact that it updates the k vectors U at each restart so that they become more and more accurate approximations of eigenvectors. On the other hand, DEFLGMRES(m,k) stops estimating eigenvectors when U is large enough so that it retains sometimes poor approximations.

Therefore, we designed a new preconditioning deflation which continuously updates the vectors in U. The new code is called DEFLATION(m,k). The strategy can be decomposed into two steps: the first step is as in DEFLGMRES and HARMONIC, indeed our algorithm still computes up to k vectors at a frequency 'freq'; the second step updates U at each restart using the strategy described below.

Let U_0 be an approximate invariant subspace of dimension k used in the current cycle. At the end of the cycle, the algorithm will compute 'freq' new vectors using the harmonic projection (3.1). After orthogonalization, we obtain a new set U_1 of $k+$ freq vectors which approximate an invariant subspace. The new deflation method updates them by solving a new generalized eigenproblem and by sorting k approximate eigenvectors. More precisely,

we solve the problem

$$(AU_1)^*(A - \theta I)U_1 u = 0$$

which is rewritten as the generalized eigenvalue problem

$$(AU_1)^* AU_1 u = \theta (AU_1)^* U_1 u, \quad U_2 = U_1 u \tag{3.2}$$

After solving this problem, we sort the k smallest eigenvalues out of $k + \text{freq}$ and orthogonalize the corresponding k vectors to get u_2 and $U_2 = U_1 u_2$. This set of orthonormal vectors U_2 is the new basis for an approximate invariant subspace of dimension k which is used to build the new preconditioner for the next cycle. We thus get the following algorithm.

Algorithm: DEFLATION(m,k)

ϵ is the tolerance for the residual norm;
convergence:= false;
choose x_0;
$M := I_n$;
$U := \{\}$;
$l := 0$;
until convergence **do**
  $r_0 = b - Ax_0$;
  Arnoldi process applied to AM^{-1} to compute V_m;
  $y_m = \text{arm argmin}_{y \in \mathbb{R}^m} \|\beta e_1 - \overline{H_m} y\|$;
  $x_m := x_0 + M^{-1} V_m y_m$;
  if $\|b - Ax_m\| < \epsilon$ convergence := true;
  else
    $x_0 = x_m$;
    estimate freq new eigenvectors U_1 of A using (3.1) ;
    $U := orthog(U, U_1)$;
    $l = l + \text{freq}$;
    if $l > k$ **do**
      compute U using (3.2) to approximate an invariant subspace of A of size k;
      $l = k$;
    endif ;
    compute $T := U^{\mathrm{T}} AU$;
    $M^{-1} := I_n + U(|\lambda_n| T^{-1} - I_l) U^{\mathrm{T}}$;
  endif
enddo

4. Numerical results

In this section numerical results will be presented that compare the methods described in the previous sections on a variety of test problems and in both a workstation and parallel computing environment. The first two classes of problems, as well as the last problem, can be considered to be somewhat artificial but have been used, in modified form, by various

authors [12,7,1] in order to investigate convergence in terms of both the spectrum and conditioning of the eigenvectors. On the other hand, Problems 3 and 4 come from real applications.

The first class of problems allows for various sets of real eigenvalues which are spaced in different arithmetic progressions in the different sets, while the second set of problems gives rise to a mixture of real eigenvalues and eigenvalues arranged on the boundary of some circle in the complex plane.

The third linear system arises when solving a biharmonic problem on a square when a B-spline (cubic basis) is used for an orthogonal collocation discretization. Some prepivoting is used for several of the last rows which correspond to the boundary points [21]. Biharmonic equations arise in a number of areas, such as the modelling of thin plate mechanics and in Stokes flow. Hermitic bicubic orthogonal collocation discretizations produce fourth-order accuracy for both uniform and non-uniform meshes. Previous techniques for solving these problems include FFTs and a direct approach [21]—which uses the fact that the problem can be represented as a coupled Poisson equation, that is, a two-block process.

The fourth problem comes from an Australian application which deals with the fitting of surfaces to various climate data gathered from the Australian continent (see [4] for more details). In particular, rainfall data from up to 6 000 irregularly scattered weather stations is processed every week in order to produce rainfall surfaces for the whole of Australia with a view to evaluating the effects of drought on agricultural production [10]. A generalized cross validation process takes place in which thin plate splines are fitted to the rainfall data. This requires the solution of a sequence of linear systems of the form

$$(A + \lambda I)y = b$$

where $\lambda > 0$ is the surface-fitting parameter, which is minimized in the GCV process [8]. While this system of equations is always positive definite as λ approaches its minimum value many of the eigenvalues are close to zero. The data set that is chosen represents 1 080 data points chosen across the state of Queensland.

The fifth problem is simply a bidiagonal matrix, in order to allow a variety of eigenvalues along with a large matrix size.

Problem 1. *Let $S(n, n_1, \beta) = (1, \beta)$ be a bidiagonal matrix of order n with 1 on the diagonal and 0 on the upper diagonal from elements 1 to n_1 and β from elements $n_1 + 1$ on, and also let $D(n, p, r)$ be a diagonal matrix of order n with values ranging from p to r in arithmetic progression. Let the system matrix of dimension n then be given by*

$$A = S(n, n_1, \beta) \begin{pmatrix} D(n_2, p, r) & 0 \\ 0 & D(n - n_2, p_1, r_1) \end{pmatrix} S(n, n_1, \beta)^{-1}$$

and the right-hand side be the unit vector. By choosing $n, n_1, n_2, p, p_1, r, r_1$ in different ways we are able to investigate the effect of various types of clustering on our adaptive algorithms. Furthermore, by allowing β to vary we are also able to investigate the effect of conditioning on the convergence of the algorithms.

The results of Problem 1 for DEFLGMRES, MORGAN, HARMONIC and our new deflation method DEFLATION are given in Figures 1–5. In what follows the notation DEFLATION(16,4), for example, will denote that a restart of 16 is used with at most four

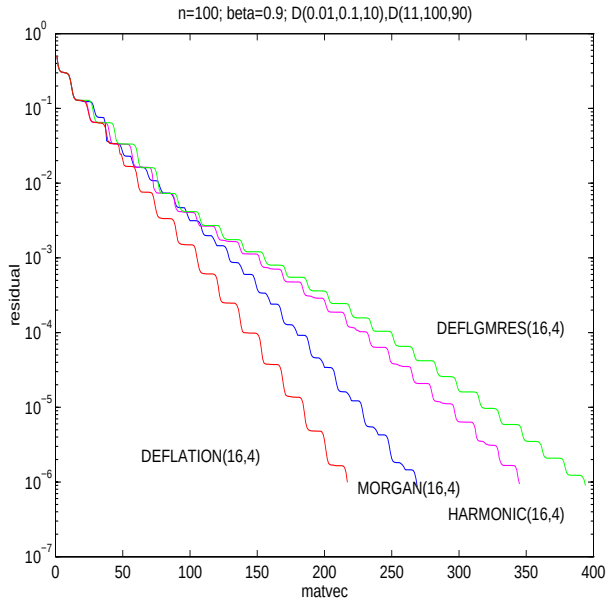

Figure 1. Comparison of implementation strategies

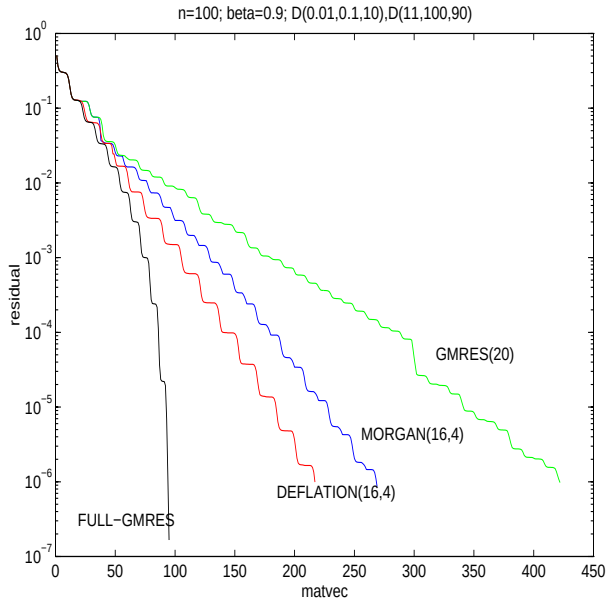

Figure 2. Comparison of full and restarted GMRES with deflation

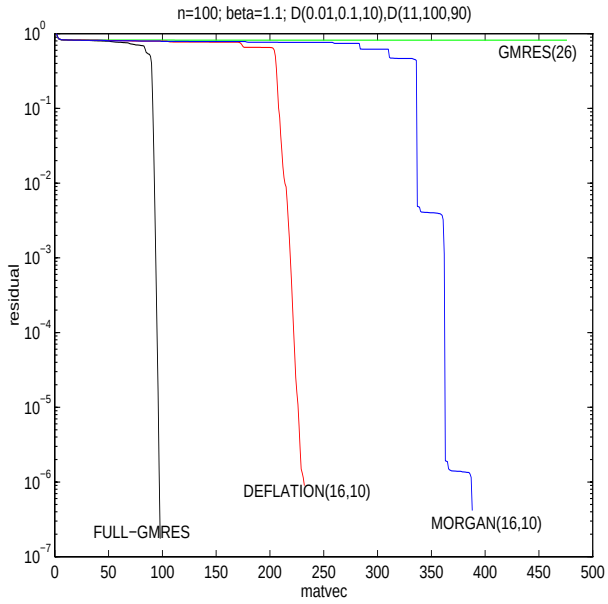

Figure 3. Convergence rates for ill-conditioned systems

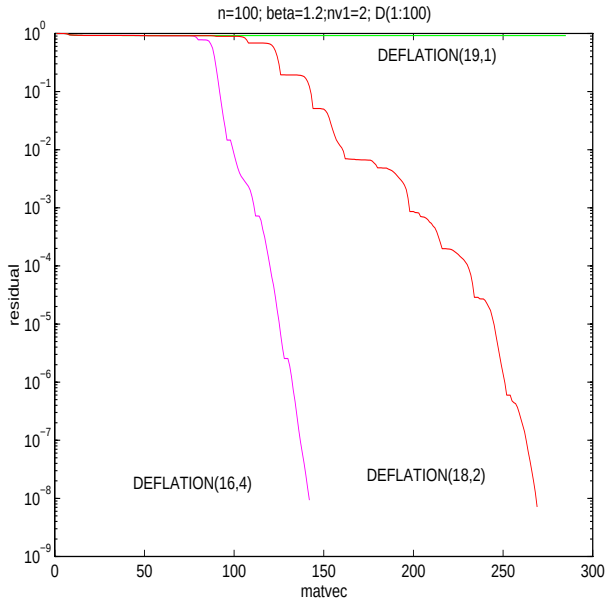

Figure 4. Convergence rates for severely ill-conditioned systems

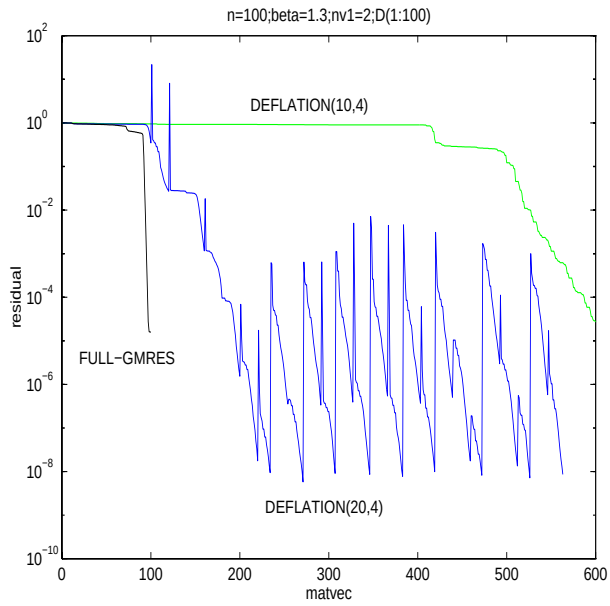

Figure 5. Convergence rates for variably coupled severely ill-conditioned systems

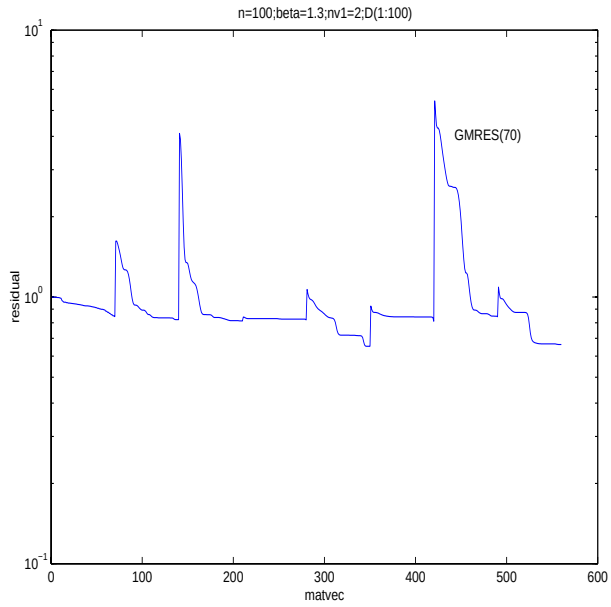

Figure 6. Convergence rate of GMRES(70) for severely ill-conditioned systems

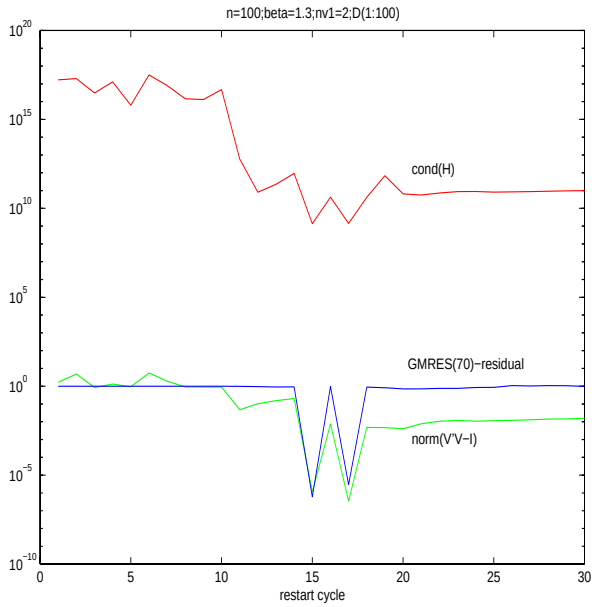

Figure 7. Residual, condition number and orthogonality for GMRES(70)

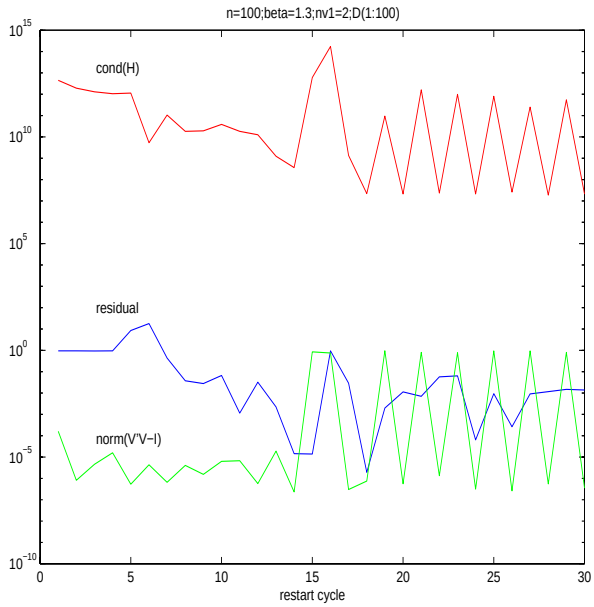

Figure 8. Residual, condition number and orthogonality for DEFLATION(20,4)

eigenvalues being deflated in total. In most cases the number of eigenvalues which can be deflated at any given time is two unless stated otherwise. It is important to recall that in all of these implementations eigenvalues are updated only after each restart.

Figure 1 essentially compares the performance of the original deflation implementation (DEFLGMRES) with the same implementation in which an harmonic estimation of the eigenvalues is used rather than the oblique projection (HARMONIC), with Morgan's method (MORGAN) and with the new deflation method (DEFLATION). For a problem of moderate size ($n = 100$) in which there is a small cluster of small eigenvalues between 0.01 and 0.1 and then a uniform distribution of larger eigenvalues, it can be seen that DEFLATION is superior to all the other methods with an improvement in efficiency of about a factor of two over the original implementation described in [7]. These results are placed in context with Full GMRES and with restarted GMRES(20) which has approximately the same memory requirements as DEFLATION(16,4) in Figure 2.

In Figure 3 the conditioning of the problem is made considerably worse by changing the value of β from 0.9 to 1.1, although the eigenvalue distribution remains the same. Figure 3 shows the effect of this ill-conditioning in that restarted GMRES with a bigger restart now fails to converge. In fact, DEFLATION(16,4) and MORGAN(16,4) also failed to converge and more eigenvalues (10) had to be deflated in order to obtain convergence. In all cases, including full GMRES, convergence was initially very slow, with DEFLATION being smoother in its convergence than MORGAN. This property of initial stalling was noticed for all methods when the system matrix was severely ill-conditioned.

Finally for Problem 1, Figure 4 shows the effects of having two subsystems in which there is a strong coupling between the two subsystems and for which the overall matrix is very ill-conditioned ($\beta = 1.2$). These results indicate that it is important to deflate at least all of the eigenvalues in the first block otherwise the ill-conditioning will cause the convergence to stall.

These effects are emphasized in Figure 5, where the same eigenvalue distribution is maintained but β is increased to 1.3, so that cond(A) is about 10^{22} and cond(S) is about 10^{12}. Some very interesting effects are observed here in that even for full GMRES it is not possible to gain a stable residue of less than approximately 10^{-5}. Another interesting effect is the peaks observed in convergence curves. With unpreconditioned GMRES(m), convergence either stalls for about $m \leq 60$ or the residuals grow in an unbounded fashion for larger m, as can be seen in Figure 6 for $m = 70$. With DEFLATION(10,4), residuals first stall then decrease rapidly but with DEFLATION(20,4) residuals show unusual peaks.

In order to explain this behaviour, we computed, after each cycle the condition number cond($\overline{H}_m$) of the Hessenberg matrix $\overline{H}_m$ defined by (2.1) for GMRES(m) and by (2.8) for DEFLATION(k,m). We also measured the loss or orthogonality in the Krylov basis with the residual $\|V_m^* V_m - I_m\|$. Figures 7 and 8 show three curves respectively, for GMRES(70) and DEFLATION(20,4) : the residual $\|r_m\| = \|b - Ax_m\|$ after each cycle, the condition number cond($\overline{H}_m$) and the orthogonality residual $\|V_m^* V_m - I_m\|$. Clearly, the quantities cond($\overline{H}_m$) and $\|V_m^* V_m - I_m\|$ are closely related. Indeed, the relation $AV_m = V_{m+1}\overline{H}_m$ implies cond(AV_m) = cond($\overline{H}_m$); since the Arnoldi method is nothing other than modified-Gram–Schmidt applied to the system (v_1, AV_m), numerical difficulties will likely happen when AV_m is ill-conditioned, as proved, for example, in [2]. Therefore, an ill-conditioned Hessenberg matrix will lead to a loss of orthogonality in V_m.

The residual $\|r_m\|$ in GMRES(70) is also strongly coupled with the two other quantities. It is not so clear for the residual $\|r_m\|$ in DEFLATION(20,4), although there is some evident relation. So, we conclude from this study that in this case a severely ill-conditioned matrix

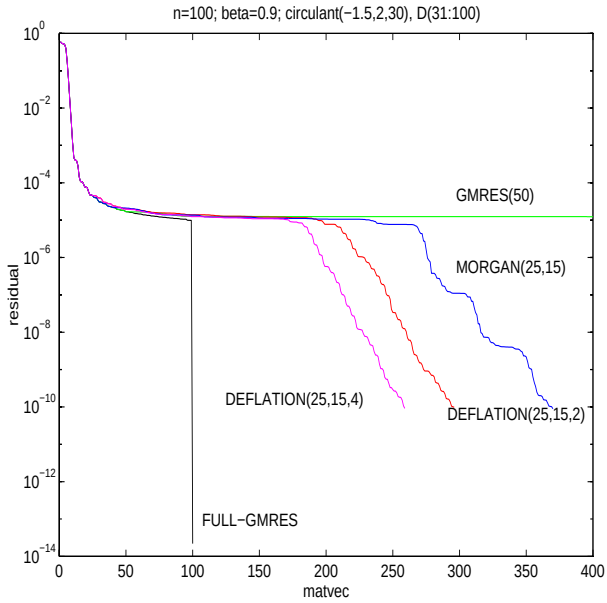

Figure 9. Convergence rates for Problem 2

A or AM^{-1} implies, in most cases, an ill-conditioned Hessenberg matrix which in turn has two numerical effects: a loss of orthogonality in V_m and an oscillating residual $\|r_m\|$.

Problem 2. *The second class of problems is one chosen from [1], with a slight modification. In this case A is given by*

$$A = S(n, n_1, \beta) \begin{pmatrix} A_{n_2} & 0 \\ 0 & B_{n-n_2} \end{pmatrix} S(n, n_1, \beta)^{-1}$$

where A_n is a circulant matrix of dimension n with first row $(c, 0, \ldots, 0, d)$ while B_n is a diagonal matrix of size n with uniformly distributed random numbers in $[a, b]$. The eigenvalues of A_n lie on a circle of centre c and radius d.

Convergence results for full GMRES, restarted GMRES, MORGAN and DEFLATION are given for Problem 2 in Figures 9 and 10. For this problem the smallest eigenvalues in magnitude are distributed evenly around a circle (in this case 30 eigenvalues in a circle of radius two and centre $-3/2$). For $n = 100$ and $\beta = 0.9$, Figure 9 shows that all methods stall at a residue of about 10^{-5} with full GMRES only converging on the last iteration. Thus, in this case restarted GMRES will prove completely inadequate while DEFLATION is again superior to MORGAN. Other numerical tests not presented here show that, in this case, deflating about half of the eigenvalues scattered around the circle gave close to optimal performance while deflating four eigenvalues at a time at each restart was superior to deflating two at a time.

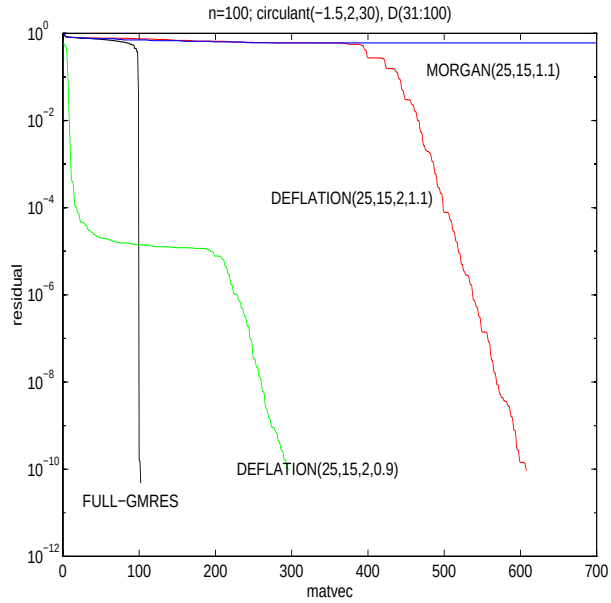

Figure 10. Convergence rates with severe ill-conditioning

Figure 10 shows that for the same eigenvalue distribution but with much greater ill-conditioning, MORGAN fails for almost all possible choices of parameters for the restart and the eigenvalue deflation, while DEFLATION is still robust. The difficulties associated with severe ill-conditioning are clearly illustrated in Figure 10 when comparing DEFLATION(25,12,2) with the β values of 0.9 and 1.1. Here the notation DEFLATION(25,12,2,1.1) means that deflation is used with a restart of 25, with 12 eigenvalues being deflated, two at a time, on a problem with $\beta = 1.1$.

Problem 3. *Problem 3 is included to show the performance of the deflation approach on an important application coming from the numerical solution of partial differential equations using collocation techniques. In this case the size of the problem is 2 048 and the system of equations is dense. An initial diagonal row scaling was applied as a preconditioner. The tests were performed on Morgan's method running on one, two and four processors of an SGI Power Challenge at the University of Queensland and the times are given in seconds. In each case the residual in the two-norm was about* 10^{-4}.

The results in Table 1 show a number of important points.

- *In terms of time MORGAN(26,4) is at least twice as fast as GMRES(30) for the same memory requirements.*
- *Full GMRES is not much faster than MORGAN.*
- *There are good parallel efficiencies between one and four processors (approximately 75%) on a shared memory parallel computer. This is due to the fact that the problem is dense and reasonably large. For sparse problems the efficiencies would be smaller.*

Table 1. Results comparing MORGAN, full and restarted GMRES

performance	FULL GMRES	MORGAN(26,4)	GMRES(30)
Iterations	57	77	1487
One processor	17.33	21.73	45.111
Two processors	9.02	11.41	—
Four processors	6.06	7.33	—

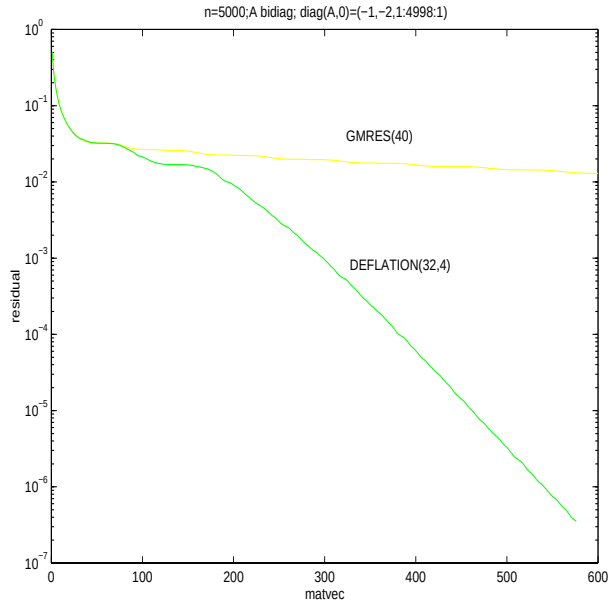

Figure 11. Convergence rates for Problem 5

Problem 4. *In this section some negative results are reported for the surface-fitting problem when λ is small. In this case the system matrix has a large number of eigenvalues clustered near zero and only a few relatively large eigenvalues. Thus, the deflating of a small number of eigenvalues gives little advantage over restarted GMRES. However, in this GCV application a number of systems of equations have to be solved which are just updated by a constant diagonal term λ. By preserving the eigenvectors across the systems, as shown in [23] and [18], deflation can work very impressively across systems of equations if special structures can be exploited (in this case the eigenvectors remain the same from system to system).*

Problem 5. *Problem 3 gives an example where MORGAN(k,m) is efficient for a large linear system. Finally, we report results on a large matrix in order to show the efficacy of DEFLATION(k,m) when the size of the Krylov subspace is much smaller than the matrix order. Let $A = (\alpha, d)$ be a bidiagonal matrix of order n with $\alpha = 0.1$ on the subdiagonal and the vector d on the main diagonal. Figure 11 shows convergence curves of the methods*

GMRES(40) and DEFLATION(32,4) for $n = 5\,000$ *and* $d = (-1, -2, 1 : 4\,998 : 1)$. *For the same memory requirements, our deflation method considerably improves the classical restarted GMRES.*

5. Conclusions

This paper has built on the previous work of [7] and [12] to develop an automatic preconditioning approach for restarted GMRES in which new eigenvalues are deflated and progressively refined in a preconditioner which is updated at each restart. This modification leads to considerable improvements over both the augmented subspace method and the original deflating preconditioner. Furthermore, this approach seems to be more robust than either of these two approaches in the face of extreme ill-conditioning of the eigenvectors. Difficulties still remain in knowing how to choose a priori the size of the restart, the total number of eigenvalues to be deflated and how many are deflated at each restart. However, the numerical results presented here show that some general strategies can be applied if a priori information is known about the spectrum and the conditioning of the eigenvectors. In any case, the deflation approach appears to be robust against possible poor choices of these parameters.

It is intended, however, to automate this choice further and to consider how this approach can be used in software where sequences of linear systems have to be solved from step to step (as in ordinary differential codes) in which much of the system information (eigenvectors, for example) is preserved form step to step.

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