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A HYBRID CHEBYSHEV KRYLOV SUBSPACE ALGORITHM FOR SOLVING NONSYMMETRIC SYSTEMS OF LINEAR EQUATIONS*

HOWARD C. ELMAN†, YOUCEF SAAD‡ AND PAUL E. SAYLOR§

Abstract. We present an iterative method for solving large sparse nonsymmetric linear systems of equations that enhances Manteuffel's adaptive Chebyshev method with a conjugate gradient-like method. The new method replaces the modified power method for computing needed eigenvalue estimates with Arnoldi's method, which can be used to simultaneously compute eigenvalues and to improve the approximate solution. Convergence analysis and numerical experiments suggest that the method is more efficient than the original adaptive Chebyshev algorithm.

Key words. iterative methods, Chebyshev methods, conjugate gradient methods, adaptive methods, nonsymmetric matrices, sparse matrices

1. Introduction. The adaptive Chebyshev algorithm of Manteuffel [11], [13] is an iterative method for solving large sparse real nonsymmetric systems of linear equations of the form

$$Ax = b, \tag{1}$$

where the coefficient matrix A has positive-definite symmetric part. Starting from an initial guess, x_0, the method generates a sequence of iterates $\{x_j\}$ whose residuals $\{r_j = b - Ax_j\}$ satisfy

$$r_j = P_j(A)r_0, \tag{2}$$

where

$$P_j(z) = T_j\left(\frac{d-z}{c}\right) \Big/ T_j\left(\frac{d}{c}\right). \tag{3}$$

T_j is the jth Chebyshev polynomial of the first kind

$$T_j(z) = \cosh\,(j \cosh^{-1}(z)),$$

and c and d are *iteration parameters* that depend on the convex hull of the spectrum of A. Two properties of the Chebyshev polynomials make this algorithm effective. First, for an appropriate choice of the iteration parameters, the residual polynomials $P_j(A)$ decrease rapidly in norm, so that the algorithm is rapidly convergent [13]. Second, the three-term recurrence for Chebyshev polynomials induces an inexpensive recurrence for the computation of each iterate x_j.

Because the iteration parameters depend on the convex hull of the spectrum of A, estimates of the extreme eigenvalues of A are needed. Manteuffel's algorithm computes these estimates dynamically [11]. It starts with a (possibly arbitrary) guess for the required parameters and monitors the convergence of the iterates generated. If convergence is deemed unsatisfactory, then information produced during the iteration

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† Department of Computer Science, University of Maryland, College Park, Maryland 20742. This work was performed while this author was at Yale University.

‡ Computer Science Department, Yale University, New Haven, Connecticut 06520.

§ Computer Science Department, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801.

is used to compute eigenvalue estimates. These, in turn, are used to compute new iteration parameters, and the Chebyshev iteration is restarted with the new parameters. This adaptive procedure is repeated until good iteration parameters are found, after which the Chebyshev method can proceed with no further adaptive steps.

The eigenvalue computation makes use of the residuals generated by the previous Chebyshev iteration. The underlying numerical method is a modified version of the power method. If the values of the iteration parameters used by the Chebyshev iteration are inaccurate, then the residuals generated may diverge. Although divergent residuals may enhance the ability of the adaptive procedure to obtain accurate eigenvalue estimates and iteration parameters, the residual norms may increase by several orders of magnitude before good iteration parameters are found [5], [7]. Thus, the adaptive Chebyshev method may do a considerable amount of work to compute iteration parameters before it makes any improvement in the accuracy of the approximate solution of the linear system.

In this paper, we present an alternative to the eigenvalue computation part of the Manteuffel algorithm that decreases the sensitivity of the Chebyshev method to iteration parameters. We replace the modified power method for computing eigenvalues with Arnoldi's method [1], [18], a generalization of the Lanczos method [16] that estimates the eigenvalues of a nonsymmetric matrix A by reducing it to upper-Hessenberg form. An advantage of this method comes from its relationship to conjugate gradient-like iterative methods for solving nonsymmetric linear systems [5], [17], [20]. At relatively little extra expense, information provided by Arnoldi's method can be used to perform several steps of an iterative method that improves the quality of the solution iterate prior to restarting the Chebyshev iteration with new parameters. The *hybrid method* combines the basic Chebyshev method with this conjugate gradient-like iteration, which is performed whenever new eigenvalue estimates are computed.

In § 2, we briefly describe the original adaptive Chebyshev method. In § 3, we describe Arnoldi's method and its relationship to conjugate gradient-like iterative methods for nonsymmetric linear systems, and we present a convergence result for one of these iterative methods. In § 4, we define the hybrid method and discuss its advantages, and in § 5, we present the results of some numerical experiments comparing the performances of the hybrid method, the adaptive Chebyshev method and the CG-like method Orthomin [4], [5], [23], [25] in solving some discretized non-self-adjoint elliptic partial differential equations.

2. The adaptive Chebyshev method. In this section, we give a brief overview of Manteuffel's adaptive Chebyshev method. For given iteration parameters c and d, the basic Chebyshev iteration is [13].

ALGORITHM 1: The Chebyshev method.

1. *Start*: Choose an initial guess x_0, compute $r_0 = b - Ax_0$ and $p_0 = (1/d)r_0$.
2. *Iterate*: FOR $j = 0$ STEP 1 UNTIL convergence DO:

$$x_{j+1} = x_j + p_j$$

$$r_{j+1} = b - Ax_{j+1}$$

$$\alpha_{j+1} = \begin{cases} 2d/(2d^2 - c^2), & j = 0 \\ [d - (c/2)^2 \alpha_j]^{-1}, & j \geqq 1 \end{cases}$$

$$\beta_{j+1} = d\alpha_{j+1} - 1$$

$$p_{j+1} = \alpha_{j+1} r_{j+1} + \beta_{j+1} p_j.$$

The cost is one matrix-vector product plus $2N$ multiplications per step. The storage required is $4N$ words for x_j, Ax_j, r_j, and p_j. The residuals $\{r_j\}$ satisfy (2) and (3), and P_j is a member of

$$\mathbf{P}_j \equiv \{\text{real polynomials of degree } j \text{ such that } P_j(0) = 1\}. \tag{4}$$

The parameters c and d define the center, d, and foci, $d \pm c$, of a family of confocal ellipses in the complex plane. There is a smallest member of this family, the *smallest ellipse*, that contains the spectrum of A. If the closure of the smallest ellipse does not contain the origin, then Algorithm 1 converges. Moreover, convergence is nearly optimum in the sense that as j increases, P_j rapidly approaches the polynomial in $\mathbf{P}_j$ with minimum uniform norm over the smallest ellipse.

If the spectrum of A lies in the right half plane, then there is an infinite number of smallest ellipses, each of which uniquely corresponds to a set of Chebyshev iteration parameters. For any particular choice of parameters, the rate of convergence of the Chebyshev iteration is [13], [22], [24]

$$-\log\left(\max_{\lambda \in \sigma(A)} S(\lambda)\right), \tag{5}$$

where

$$S(z) = S_{c,d}(z) = \frac{d - z + [(d-z)^2 - c^2]^{1/2}}{d + [d^2 - c^2]^{1/2}}. \tag{6}$$

The iteration count for convergence is (approximately) proportional to the reciprocal of the rate of convergence. Hence, the *best ellipse* is defined to be that smallest ellipse for which the rate of convergence is greatest. The adaptive Chebyshev method starts with (possibly arbitrary) initial values for the iteration parameters and monitors the convergence of the Chebyshev iteration (Algorithm 1). If convergence is deemed unsatisfactory (i.e. the residuals are diverging or converging less rapidly than (5) suggests) after step s, then the adaptive procedure

1. estimates eigenvalues on the convex hull of the spectrum of A [11], and
2. computes the iteration parameters for the best ellipse containing these eigenvalue estimates [13].

The Chebyshev iteration is then restarted with the new parameters. The adaptive procedure is repeated as often as is deemed necessary, until good parameters are found, after which the Chebyshev iteration is performed until convergence.

The second step of the adaptive procedure, the computation of iteration parameters, requires negligible machine resources, and we omit a discussion of it here.

The eigenvalue estimates are computed by a *modified power method*, which is based on the fact that, asymptotically,

$$P_j(z) \approx S(z)^j,$$

so that

$$r_j \approx S(A)^j r_0,$$

where $S(A)$ is the linear operator induced by $S(z)$. That is, the residuals resemble the vectors generated by the power method for $S(A)$. If, for given iteration parameters, some eigenvalue of $S(A)$ has modulus greater than one and r_0 has a component in the corresponding eigenvector, then the residuals will diverge but will eventually become rich in that eigenvector. If there are m such eigenvalues, then eventually the sequence of $m+1$ residuals

$$\{r_s, r_{s+1}, \cdots, r_{s+m}\}$$

will be nearly linearly dependent. Estimates for m eigenvalues of $S(A)$ are then given by the roots of the mth-degree polynomial

$$\alpha_1+\alpha_2 z+\cdots+\alpha_m z^{m-1}+z^m,$$

whose coefficients $\{\alpha_j\}_{j=1}^m$ are the solution to the least squares problem

$$\min \|[r_s, \cdots, r_{s+m-1}]\alpha + r_{s+m}\|_2, \tag{7}$$

where $[r_s, \cdots, r_{s+m-1}]$ denotes the matrix with columns $\{r_j\}_{j=s}^{s+m-1}$ and α denotes the vector whose jth component is α_j[11]. Estimates for eigenvalues of A can be computed from the relationship

$$\mu = S(\lambda)$$

between eigenvalues $\{\mu\}$ of $S(A)$ and $\{\lambda\}$ of A.

Hence, the modified power method consists of m Chebyshev steps to generate the residuals $\{r_j\}_{j=s+1}^{s+m}$, followed by the computation of the least squares solution to (7), and the computation of new eigenvalue estimates and iteration parameters. The Chebyshev steps require m matrix-vector products and $2mN$ multiplications. If (7) is solved using the normal equations, then $[(m^2+3m)/2]N$ multiplications are needed to compute the inner products

$$(r_{s+j}, r_{s+k}), \quad 0 \leqq j \leqq m-1, \quad 0 \leqq k \leqq m. \tag{8}$$

Therefore, the dominant cost is m matrix-vector products plus $[(m^2+7m)/2]N$ additional multiplications. The storage requirement (over that of the Chebyshev iteration) is mN words to save the vectors $\{r_{s+j}\}_{j=1}^m$.

Note that an "unmodified" power method could be used instead of the modified power method by replacing $\{r_{s+j}\}_{j=1}^m$ with $\{A^j r_s\}_{j=1}^m$ in (7) [11]. We will examine a technique that is mathematically equivalent to the unmodified power method in § 3.

3. Arnoldi's method and its relation to iterative linear solvers. In this section, we describe Arnoldi's method for computing eigenvalues of nonsymmetric matrices, show how it can be used as the basis for iterative methods for solving linear systems, and derive a convergence bound for one of these linear solvers.

Given an arbitrary vector v_1 such that $\|v_1\|_2 = 1$, Arnoldi's method [1], [18] is a Galerkin method on the Krylov subspace $K_m = \text{span}\{v_1, Av_1, \cdots, A^{m-1}v_1\}$ for approximating the eigenvalues of A. That is, it finds a set of eigenvalue estimates $\{\lambda_1, \cdots, \lambda_m\}$ such that there exist nonzero $u_i \in K_m$, $i = 1, \cdots, m$, for which

$$(Au_i - \lambda_i u_i, v) = 0, \ i = 1, \cdots, m \tag{9}$$

for all $v \in K_m$. It accomplishes this by constructing an orthonormal matrix $V_m = [v_1, \cdots, v_m]$ whose columns $\{v_j\}_{j=1}^m$ span K_m, and then computing the eigenvalues of $V_m^T A V_m$.

ALGORITHM 2: Arnoldi's method.

1. *Start*: Choose an initial vector v_1 such that $\|v_1\|_2 = 1$, and a step number m.
2. *Iterate*: FOR $j = 1$ STEP 1 UNTIL m DO

$$h_{ij} = (Av_j, v_i), \ i = 1, \cdots, j$$

$$\hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{ij} v_i$$

$$h_{j+1,j} = \|\hat{v}_{j+1}\|_2$$

$$v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}.$$

Notice that this method is essentially a Gram-Schmidt process for orthonormalizing the Krylov sequence $\{v_1, Av_1, \cdots, A^{m-1}v_1\}$. In a practical implementation, it is usually more suitable to use a modified Gram-Schmidt process. The orthonormal matrix V_m is such that $V_m^T A V_m = H_m$, where H_m is the $m \times m$ upper-Hessenberg matrix whose (i, j) entry is the scalar h_{ij}. The method generalizes the symmetric Lanczos algorithm to nonsymmetric matrices. Recall that in the symmetric case, H_m is symmetric and tridiagonal [16].

In an implementation, it is not necessary to compute the normalized vectors $\{v_j\}$; it suffices to compute and save the norms $\{\|\hat{v}_j\|_2\}$. It is also not necessary to compute $\hat{v}_{m+1}$. With these conventions, the cost of Arnoldi's method is m matrix-vector products and $(m^2+m)N$ multiplications. The storage requirement is $(m+1)N$ words for $\{v_j\}_{j=1}^m$ and Av [20].

Suppose now that x_0 is a guess to the solution of (1), with residual $r_0 = b - Ax_0$. Let $K_m = \text{span}\{r_0, Ar_0, \cdots, A^{m-1}r_0\}$. One way to solve (1) iteratively is to compute an approximate solution $x_m \in x_0 + K_m$ such that the Galerkin condition

$$(r_m, v) = 0, \qquad v \in K_m \tag{10}$$

holds. But if $v_1 = r_0/\|r_0\|_2$, then the Arnoldi vectors $\{v_j\}_{j=1}^m$ span K_m, so that

$$x_m = x_0 + V_m y_m,$$
$$r_m = r_0 - Az_m = \|r_0\|_2 v_1 - AV_m y_m,$$

for some $y_m \in \mathbf{R}^m$. Since the Arnoldi vectors are orthonormal, (10) is imposed by computing

$$y_m = H_m^{-1}\|r_0\|_2 e_1,$$

where e_j is the jth unit vector in $\mathbf{R}^m$. Hence, the algorithm [17] follows.

ALGORITHM 3: The full orthogonalization method (FOM).

1. *Start*: Choose an initial guess x_0, compute $r_0 = b - Ax_0$ and $v_1 = r_0/\|r_0\|_2$.
2. *Iterate*: Perform m steps of Algorithm 2 starting with v_1.
3. *Form the solution*:

$$\text{Solve } H_m y_m = \|r_0\|_2 e_1,$$
$$\text{compute } x_m = x_0 + V_m y_m,$$

where V_m and H_m are determined by Arnoldi's method.

Algorithm 3 is also referred to as Arnoldi's method for solving linear systems. It is theoretically equivalent to the ORTHORES method developed by Young and Jea [25], which is modelled after a version of the conjugate gradient method described by Engeli et al. [8].

A drawback of Algorithm 3 is that the approximate solution x_m does not satisfy an optimality property. An alternative is the generalized minimal residual method (GMRES) developed by Saad and Schultz [20], which uses the Arnoldi basis to compute the point $x_m \in x_0 + K_m$ whose residual norm $\|b - Ax_m\|_2$ is minimum. Let $v_1 = r_0/\|r_0\|_2$, let $\beta = \|r_0\|_2$, and let $\tilde{H}_m$ denote the $(m+1) \times m$ matrix obtained by appending to H_m a row with single nonzero entry $h_{m+1,m}$ in column m. Then the Arnoldi basis matrices V_m and $V_{m+1} = [v_1, \cdots, v_{m+1}]$ satisfy

$$AV_m = V_{m+1}\tilde{H}_m. \tag{11}$$

The GMRES iterate is given by x_0+z, where z is the solution of the least squares problem

$$\min_{z\in K_m} \|b-A(x_0+z)\|_2 = \min_{z\in K_m} \|r_0-Az\|_2 = \min_{y\in R^m} \|\beta v_1 - AV_m y\|_2. \tag{12}$$

Using (11) and the fact that V_{m+1} is orthonormal, the last expression in (12) is equal to

$$\min_{y\in R^m} \|\beta V_{m+1}e_1 - V_{m+1}\tilde{H}_m y\|_2 = \min_{y\in R^m} \|\beta e_1 - \tilde{H}_m y\|_2. \tag{13}$$

Hence, the GMRES iterate is given by $x_0+V_m y_m$, where y_m is the solution to the upper-Hessenberg least squares problem on the right-hand side of (13).

ALGORITHM 4: The generalized minimal residual method.

1. *Start*: Choose an initial guess x_0, compute $r_0=b-Ax_0$ and $v_1=r_0/\|r_0\|_2$, set $\beta=\|r_0\|_2$.
2. *Iterate*: Perform m steps of Algorithm 2 starting with v_1.
3. *Form the solution*: Find y_m minimizing $\|\beta e_1-\tilde{H}_m y\|_2$ and compute $x_m=x_0+V_m y_m$, where V_m and $\tilde{H}_m$ are determined by Arnoldi's method.

GMRES is a generalization of the MINRES algorithm presented by Paige and Saunders [15]. It is mathematically equivalent to Young and Jea's ORTHODIR [25], for arbitrary nonsingular matrices A. For matrices with positive-definite symmetric part, it is also equivalent to the generalized conjugate residual method [4], [5] and a method of Axelsson [2]. For large step numbers, it requires one third the multiplications and one half the storage of these methods [20].

For both FOM and GMRES, once $\{v_j\}_{j=1}^m$ and H_m are computed, the dominant cost of computing x_m is mN multiplications. Hence, the cost of both methods is m matrix-vector products plus $(m^2+2m)N$ multiplications. In addition to storage for x_j, $(m+1)N$ words are needed for the Arnoldi computation. We remark that for both methods, the residual norm $\|b-Ax_m\|_2$ can be monitored during Step 2 without explicitly computing x_m, so that Step 2 can be stopped as soon as the approximate solution is sufficiently accurate [20].

An error analysis of GMRES can be found in [20]. We derive a new result here that will demonstrate its effectiveness in the hybrid method. Note that the residual $r_m=b-Ax_m$ satisfies

$$\|r_m\|_2 = \min_{P_m\in \mathbf{P}_m} \|P_m(A)r_0\|_2,$$

where $\mathbf{P}_m$ is defined by (4). Assume that A is diagonalizable,

$$A = U\Lambda U^{-1}, \tag{14}$$

where Λ is the diagonal matrix of eigenvalues $\{\lambda_j\}_{j=1}^N$ and $U=[u_1,\cdots,u_N]$ is the matrix of eigenvectors of A. Note that U and Λ may be complex. Suppose that the initial residual is dominated by m eigenvectors, i.e.

$$r_0 = \sum_{j=1}^m \alpha_j u_j + e, \tag{15}$$

where $\|e\|_2$ is small in comparison to $\|\sum_{j=1}^m \alpha_j u_j\|_2$, and that, moreover the sum in (15) satisfies

(16) if some complex u_k appears in $\sum_{j=1}^m \alpha_j u_j$, then its conjugate $\bar{u}_k$ appears also.

(In general, this might require including small components in the sum, with a corresponding increase in m.)

THEOREM 1. *If A is diagonalizable and the initial residual satisfies* (15)-(16), *then the residual norm after m steps of* GMRES *satisfies*

$$\|r_m\|_2 \leqq \|U\|_2 \|U^{-1}\|_2 c_m \|e\|_2,$$

where $c_m = \max_{k>m} \prod_{j=1}^{m} |(\lambda_k - \lambda_j)/\lambda_j|$.

Proof. Let $U_m = [u_1, \cdots, u_m]$, $\Lambda_m = \operatorname{diag}(\lambda_1, \cdots, \lambda_m)$, and $a = (\alpha_1, \cdots, \alpha_m)^T$, so that (15) is equivalent to

$$r_0 = U_m a + e.$$

Consider the polynomial

$$\tilde{P}_m(z) = \prod_{j=1}^{m} \frac{z - \lambda_j}{-\lambda_j},$$

which satisfies $\tilde{P}_m(\lambda_j) = 0$, $1 \leqq j \leqq m$, $\tilde{P}_m(0) = 1$. Hence

$$\tilde{P}_m(A) U_m = U_m \tilde{P}_m(\Lambda_m) = 0,$$

so that

$$\tilde{P}_m(A) r_0 = \tilde{P}_m(A) U_m \alpha + \tilde{P}_m(A) e = \tilde{P}_m(A) e.$$

Moreover, by (16), $\tilde{P}_m$ has real coefficients so that

$$\|r_m\|_2 = \min_{P_m \in \mathcal{P}_m} \|P_m(A) r_0\|_2 \leqq \|\tilde{P}_m(A) e\|_2$$

$$\leqq \|U\|_2 \|U^{-1}\|_2 \|\tilde{P}_m(\tilde{\Lambda}_m)\|_2 \|e\|_2,$$

where $\tilde{\Lambda}_m = \operatorname{diag}(\lambda_{m+1}, \cdots, \lambda_N)$. The assertion then follows with

$$c_m = \|\tilde{P}_m(\tilde{\Lambda}_m)\|_2 = \max_{k>m} |\tilde{P}_m(\lambda_k)|. \tag{17}$$

Q.E.D.

Note that the constant c_m *does* depend on $\{\lambda_j\}_{j=1}^m$, and it may not be small if, for example, these eigenvalues are small relative to the others. However, suppose $\{\lambda_j\}_{j=1}^m$ are the m dominant eigenvalues of A (i.e. $|\lambda_j| \geqq |\lambda_k|$ for $j \leqq m$, $k > m$). Then

$$|\lambda_k - \lambda_j| \leqq 2|\lambda_j|$$

for $k > m$, so that

$$c_m \leqq 2^m.$$

Moreover, if $\{\lambda_j\}_{j=1}^m$ are large relative to the remaining eigenvalues, then typically

$$|\lambda_k - \lambda_j| \leqq |\lambda_j|. \tag{18}$$

Similarly, let $\lambda_j = \mu_j + i\nu_j$, $\lambda_k = \mu_k + i\nu_k$. Then

$$\left|\frac{\lambda_k - \lambda_j}{\lambda_j}\right|^2 \leqq \left(1 - \frac{\mu_k}{\mu_j}\right)^2 + \frac{(\nu_j - \nu_k)^2}{\mu_j^2 + \nu_j^2},$$

which is less than one if λ_j and λ_k are real, and will typically be of order one if their imaginary parts ν_j, ν_k are small. In all these cases, c_m will be of order one, and the m steps of GMRES reduce the residual norm to the order of $\|e\|_2$ provided that the condition number of U is not too large. Finally, the possibility that c_m may be large is really only a problem if the bound of the theorem is sharp. But in that case, the polynomial used in the proof is nearly optimal, and therefore $\|e\|_2$ is very small.

4. The hybrid method. The hybrid method combines the approaches of the previous two sections. It uses the basic Chebyshev iteration of Algorithm 1, but replaces the modified power method for computing eigenvalues with Arnoldi's method, from which information is also used to improve the solution iterate. Either FOM or GMRES could be used for the solution update; we favor GMRES because of its minimization property. In the following implementation, the convergence of the Chebyshev iteration is monitored by examining the norms of the generated residuals, and the adaptive procedure is invoked if the residual norm exceeds a specified tolerance r relative to the norm of $r_{\min} = r_{\min}(c, d)$, the smallest residual encountered with the current iteration parameters. In addition, the adaptive procedure is invoked periodically, after at most s Chebyshev steps, and it is used to generate initial eigenvalue estimates from which initial iteration parameters are obtained.[1]

ALGORITHM 5: The hybrid method.
Choose x_0. Compute $r_0 = b - Ax_0$.
UNTIL Convergence DO
Adaptive Steps: Set $v_1 =$ the current normalized residual, perform m Arnoldi/GMRES steps (Algorithm 4), and use the new eigenvalue estimates to update (or initialize) the iteration parameters.
Chebyshev Steps: Set $j_{\max} = j + s$.
WHILE ($\|r_j\|_2 / \|r_{\min}\|_2 \leqq r$ and $j+1 \leqq j_{\max}$)
Compute x_{j+1} by the Chebyshev iteration.

The Chebyshev step requires one matrix-vector product and $2N$ multiplications per iteration, and the adaptive step requires m matrix-vector products and $(m^2+2m)N$ multiplications. As with the modified power method, the eigenvalue estimates provided by Arnoldi's method lie in the field of values of A but not necessarily in the convex hull of the spectrum of A, so that the hybrid method is only rigorously applicable to linear systems with positive-definite symmetric part. The storage requirement for the adaptive step is mN words, the same as for the modified power method, since the first Arnoldi vector can share storage with the residual of the Chebyshev iteration.

There are two main differences between the original adaptive Chebyshev method and the hybrid method:

1. Different eigenvalue computations: the adaptive Chebyshev method uses the modified power method based on the operator $S(A)$, whereas the hybrid method uses Arnoldi's method, which is based on a Krylov subspace in A.

2. Purification: the hybrid method uses the GMRES steps to improve the approximate solution.

A third difference is that in the hybrid method, the initial eigenvalue estimates provided by Arnoldi's method can be used to compute initial iteration parameters; the original Chebyshev method requires an initial guess.

We do not know whether the use of Arnoldi's method alone offers any advantage, i.e. whether Arnoldi's method provides more accurate eigenvalue estimates than the modified power method. Arnoldi's method is mathematically equivalent to the "unmodified" power method discussed by Manteuffel [11], who observed no significant difference between the unmodified and modified methods. Numerical experiments comparing the two techniques are described in § 5.

[1] Manteuffel's method [13] for computing iteration parameters from eigenvalue estimates is still used.

The effect of the GMRES steps can be explained by a heuristic analysis based on Theorem 1. Assume that A is diagonalizable as in (14). If the initial residual for the hybrid method has the form

$$r_0 = \sum_{j=1}^{N} \gamma_j u_j,$$

then after s Chebyshev iterations, the residual is approximately equal to [13]

$$\tilde{r} = \sum_{j=1}^{N} \tau_j^s \gamma_j u_j, \tag{19}$$

where

$$\tau_j = S(\lambda_j) = \frac{d - \lambda_j + [(d-\lambda_j)^2 - c^2]^{1/2}}{d + [d^2 - c^2]^{1/2}},$$

and c, d are the iteration parameters used in the Chebyshev step. Suppose that these parameters are inaccurate, so that the components in the directions of some eigenvectors are not being damped out. This means that some of the $\{\tau_j\}$ satisfy $|\tau_j| > 1$, so that $|\tau_j^s| \gg 1$ and the terms with these coefficients dominate (19). Note that $|\tau_j| = |\bar{\tau}_j|$, so that if some complex eigenvector is not being damped out, then neither is its conjugate. For some m, therefore, $\tilde{r}$ satisfies (15) (with $\alpha_j = \tau_j^s \gamma_j$) and (16). If the corresponding eigenvalues $\{\lambda_j\}$ of A are the dominant ones, then Theorem 1 suggests that the m GMRES steps *purify* the residual of the eigenvectors whose coefficients had been growing during the Chebyshev iteration. Moreover, since $\tilde{r}$ is the starting vector for the Arnoldi computation and is presumably rich in these eigenvectors, the new eigenvalue estimates will be good approximations to the corresponding eigenvalues. Hence, the new iteration parameters will produce Chebyshev polynomials that continue to damp out these components.

Although the correct value of m to use in the adaptive step is not known in general, this analysis still shows that m GMRES steps will tend to damp out the m dominant components of (19). The analysis applies as well even if the iteration parameters are accurate but not optimal, i.e. the Chebyshev iteration is damping out all components but better parameters exist. In this case, some components will not be damped out as rapidly as others during the Chebyshev step, and these will eventually be dominant in (19).

Since the purification step seems to provide the important advantage of the hybrid method, it is natural to ask whether a similar idea can be implemented with the modified power method, which uses $\{r_{s+j} \approx S(A)^{s+j} r_0\}_{j=0}^{m}$ to compute eigenvalue estimates. One such procedure consists of computing

$$\tilde{x} \in x_{s+m} + \text{span}\{r_s, \cdots, r_{s+m-1}\} \tag{20}$$

for which $\|\tilde{r}\|_2 = \|b - A\tilde{x}\|_2$ is minimum. This requires the solution of the least squares problem

$$\min \|r_{s+m} - \sum_{j=0}^{m-1} \alpha_j A r_{s+j}\|_2. \tag{21}$$

To solve (21) using the normal equations, it is necessary to compute the inner products

$$(Ar_{s+j}, Ar_{s+k}), \qquad 0 \leqq j \leqq k \leqq m-1, \tag{22}$$

$$(r_{s+m}, Ar_{s+j}), \qquad 0 \leqq j \leqq m-1. \tag{23}$$

Note that the recurrence for the Chebyshev iteration induces a three-term residual recurrence

$$Ar_j = -\frac{\beta_j}{\alpha_j} r_{j-1} + \frac{1+\beta_j}{\alpha_j} r_j - \frac{1}{\alpha_j} r_{j+1}. \tag{24}$$

Therefore, except when $j=0$, all the quantities of (22) can be computed in terms of

$$(r_{s+t}, r_{s+u}), \qquad t = j-1, j, j+1, \quad u = k-1, k, k+1,$$

which are available from the modified power method (see (8) above). Similarly, except when $j=0$ and $j=m-1$, the terms of (23) are available from the modified power method. Moreover, the same trick can be used for $j=0$ in (22) if r_{s-1} is saved and $\{(r_{s-1}, r_{s+k})\}_{k=-1}^{m-1}$ are computed; and for $j=0$ and $j=m-1$ in (23) if (r_{s-1}, r_s) and (r_{s+m}, r_{s+m}) are computed. Hence (21) can be solved with a total of $m+3$ inner products. The computation of $\tilde{x}$ requires an additional mN multiplications, so that purification can be added to the modified power method with $(2m+3)N$ multiplications. Combining this with the $[(m^2+7m)/2]N$ multiplications and m matrix-vector products required for the modified power method, the cost of this adaptive procedure is m matrix-vector products plus $[(m^2+11m+6)/2]N$ multiplications. This contrasts with m matrix-vector products and $(m^2+2m)N$ multiplications for the hybrid method. Thus, the number of matrix-vector products is the same as for the hybrid method, but the number of additional operations is different. The coefficient of N for the additional operation counts of both methods, for several values of m, is shown in Table 4.1. The storage requirement is $(m+1)N$ words, for $\{r_{s+j}\}_{j=1}^{m}$ and r_{s-1}, which is N greater than for the hybrid method.[2]

TABLE 4.1
Coefficient of N in multiplication count of purification adaptive steps.

	m	2	4	6	8	10
Hybrid		8	24	48	80	120
Modified power with purification		16	33	54	79	108

Finally, we note that similar methods for annihilating eigencomponents have been developed in slightly different contexts by Saad and Sameh [19] and by Jesperson and Buning [10].

5. Numerical experiments. In this section, we describe the results of numerical experiments in which the methods discussed above are used to solve some nonsymmetric linear systems arising from the discretization of non-self-adjoint elliptic boundary value problems. We examine four methods based on four choices for the adaptive procedure:

(A) CHEB: the modified power method with no purification;
(B) HYBRID: Arnoldi's method with purification by GMRES;
(C) CHEB-MIN: the modified power method with purification added by solving (21);
(D) CHEB-ARNOLDI: Arnoldi's method *without* purification.

[2] Note that the space in (20) does not contain the most recent information available, since r_{s+m} is excluded. We exclude it to avoid the computation of Ar_m in (21). Also, a less expensive purification, with no reference to r_{s-1}, could be performed if r_s were excluded. The given method is a compromise between these two alternatives.

The experiments were run on a VAX11-780 in double precision (55 bit mantissa). The Chebyshev iterations were based on a slightly modified version of Manteuffel's Chebyshev code [12]. The eigenvalues of the upper-Hessenberg matrix H_m generated by Arnoldi's method were computed using EISPACK [21].

Table 5.1 summarizes the work and storage requirements for the adaptive procedures of each of the four methods. The matrix-vector products are denoted by Av.

TABLE 5.1
Work and storage requirements for the adaptive procedures.

	CHEB	HYBRID	CHEB-MIN	CHEB-ARNOLDI
Work	$mAv+(m^2+7m)N/2$	$mAv+(m^2+2m)N$	$mAv+(m^2+11m+6)N/2$	$mAv+(m^2+m)N$
Storage	mN	mN	$(m+1)N$	mN

As in Algorithm 5, the adaptive procedure of each method is invoked if

$$\|r_i\|_2 > \tau \|r_{\min}\|_2, \tag{25}$$

where $r_{\min}$ is the smallest residual encountered for the current parameters, and $\tau = 2$.[3] For HYBRID and CHEB-MIN, it is also invoked after at most $s = 20$ Chebyshev steps so that the purification step is performed periodically. Since no purification occurs in CHEB and CHEB-ARNOLDI, these techniques allow the Chebyshev iteration to proceed if the convergence seems to agree with the predicted rate of convergence.[4] HYBRID and CHEB-ARNOLDI compute initial values for the iteration parameters c and d from eigenvalue estimates provided by Arnoldi's method applied to the initial residual. CHEB and CHEB-MIN use $c = 0$ and $d = 1$ as the initial iteration parameters. Following [11], we use $m = 4$ as the size of the Arnoldi and modified power bases in an effort to identify the dominant and subdominant complex eigenvalue pair. Table 5.2 contains the work and storage costs of the adaptive procedures for this value of m.

TABLE 5.2
Costs of the adaptive procedures, $m = 4$.

	CHEB	HYBRID	CHEB-MIN	CHEB-ARNOLDI
Work	$4Av+22N$	$4Av+24N$	$4Av+33N$	$4Av+20N$
Storage	$4N$	$4N$	$5N$	$4N$

For the test problem, we use the elliptic partial differential equation

$$-(e^{-xy}u_x)_x-(e^{xy}u_y)_y+\gamma[(x+y)u_y+((x+y)u)_y]+[1/(1+x+y)]u=f, \tag{26}$$

where γ is a real scalar parameter and the right-hand side f is chosen so that the solution is

$$u(x, y) = x\, e^{xy} \sin(\pi x) \sin(\pi y).$$

[3] CHEB and CHEB-MIN make this test only if i is a multiple of $m = 4$. This convention is taken from the Chebyshev code and may slightly enhance the modified power method by allowing greater residual growth than indicated by (25).

[4] If j is the index of the first Chebyshev iterate corresponding to the current iteration parameters, then asymptotically $\|r_{j+t}\|_2/\|r_j\|_2$ is bounded by $\max S(|\lambda|)^t$ for $\lambda \in \sigma(A)$ [13]. The heuristic, built into the original code [12], is to compute new parameters only if $\|r_{j+t}\|_2/\|r_j\|_2 > 2S(d)^t$.

We pose (26) on the unit square $\{0 \leqq x, y \leqq 1\}$ with homogeneous Dirichlet boundary conditions and discretize using the five-point second order centered finite difference scheme on a uniform 47×47 grid, producing a linear system

$$Ax = b \tag{27}$$

or order $N = 2209$. We use the values $\gamma = 5$ and $\gamma = 50$. In addition, we *precondition* (27) with incomplete factorizations. We use both the incomplete LU (ILU) and modified incomplete LU (MILU) factorizations with no extra fill-in (see [3], [5], [9], [14] for the details concerning these techniques). The actual linear systems on which the various iterative methods are tested have the form

$$\tilde{A}\tilde{x} = [AQ^{-1}][Qx] = b = \tilde{b},$$

where Q is the *preconditioning matrix*. We thus have four test problems:

- Problem 1: $\gamma = 5$, ILU preconditioning,
- Problem 2: $\gamma = 5$, MILU preconditioning,
- Problem 3: $\gamma = 50$, ILU preconditioning,
- Problem 4: $\gamma = 50$, MILU preconditioning.

The eigenvalue estimates (computed by all four methods) are real in Problems 1 and 2, and have imaginary parts of order one in Problems 3 and 4. For all tests, the initial guess is $x_0 = 0$ and the stopping criterion is $\|r_i\|_2 / \|r_0\|_2 < 10^{-}$.

Table 5.3 shows the number of iterations required to satisfy the stopping criterion, where an iteration for the four adaptive Chebyshev methods is defined to be either a Chebyshev step or an Arnoldi step. Thus, one iteration does not correspond to a fixed amount of work, although each iteration contains one matrix-vector product.

TABLE 5.3
Iterations to convergence.

	CHEB	HYBRID	CHEB-MIN	CHEB-ARNOLDI	ORTHO-MIN(1)
Problem 1	90	60	64	77	78
Problem 2	35	27	34	44	32
Problem 3	36	42	31	59	32
Problem 4	33	27	31	34	21

Figures 5.1–5.4 show the performance of the methods on each of the four problems. The coordinates are residual norm $\|r_i\|_2$ (on a logarithmic scale) vs. multiplications. As a benchmark, for each problem we also include the performance of the conjugate gradient-like method Orthomin (1) [4], [5], [23], [25]. Note that numerical experiments indicating that Chebyshev methods (as well as Orthomin) are more effective than the conjugate gradient method applied to the normal equations and the biconjugate gradient method are presented in [5], [6], [7].

In examining this data, we consider three main issues:

1. the effect of the purification steps in HYBRID and CHEB-MIN;
2. the effect of the different eigenvalue estimators: Arnoldi's method in HYBRID and CHEB-ARNOLDI vs. the modified power method in CHEB and CHEB-MIN;

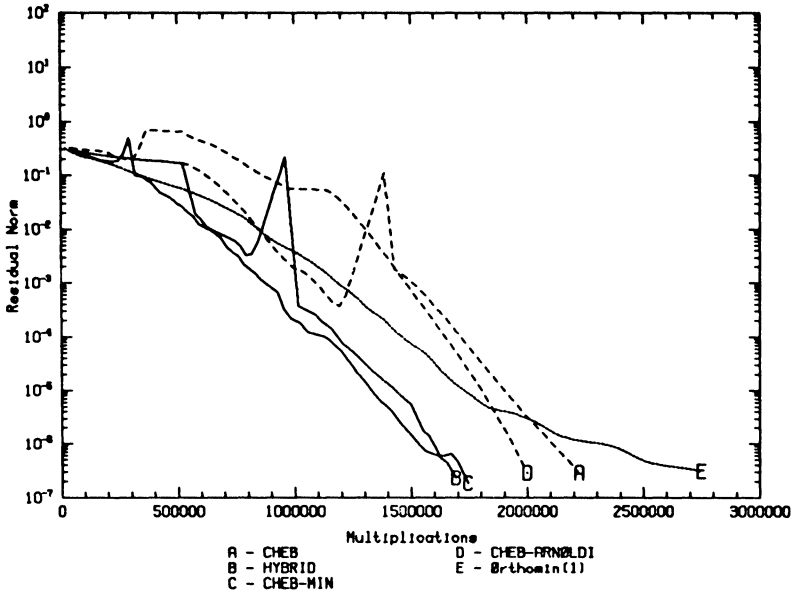

FIG. 5.1. *Problem* 1: $\gamma = 5$, ILU *preconditioning.*

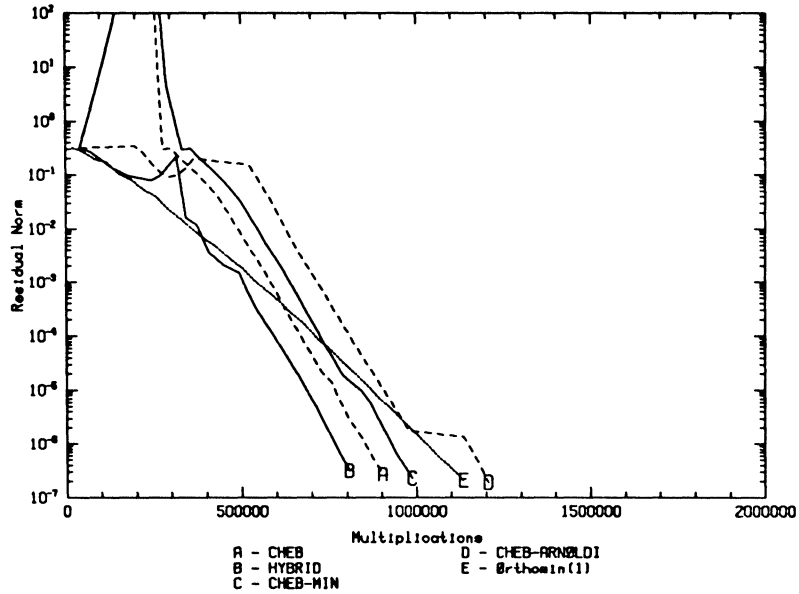

FIG. 5.2. *Problem* 2: $\gamma = 5$, MILU *preconditioning.*

3. the different choice of initial parameters: an initial Arnoldi computation in HYBRID and CHEB-ARNOLDI vs. initial guesses of $d = 1$, $c = 0$ in CHEB and CHEB-MIN.

The first issue is clearcut: for all four problems, the method with purification is superior to its analogue without purification. This is explained by the analysis of § 4: if the residuals from the Chebyshev steps are diverging, then the purification essentially annihilates the eigenvector components that are growing, at relatively little extra cost.

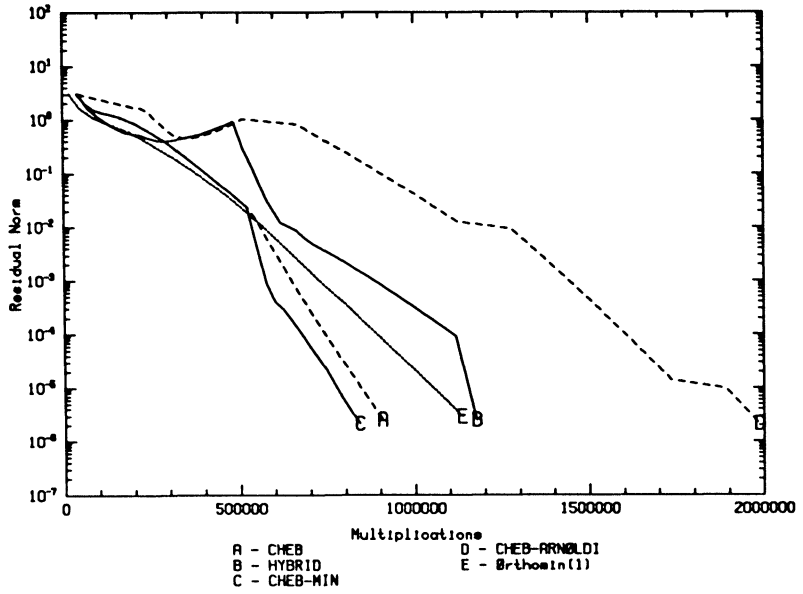

FIG. 5.3. *Problem* 3: $\gamma = 50$, ILU *preconditioning.*

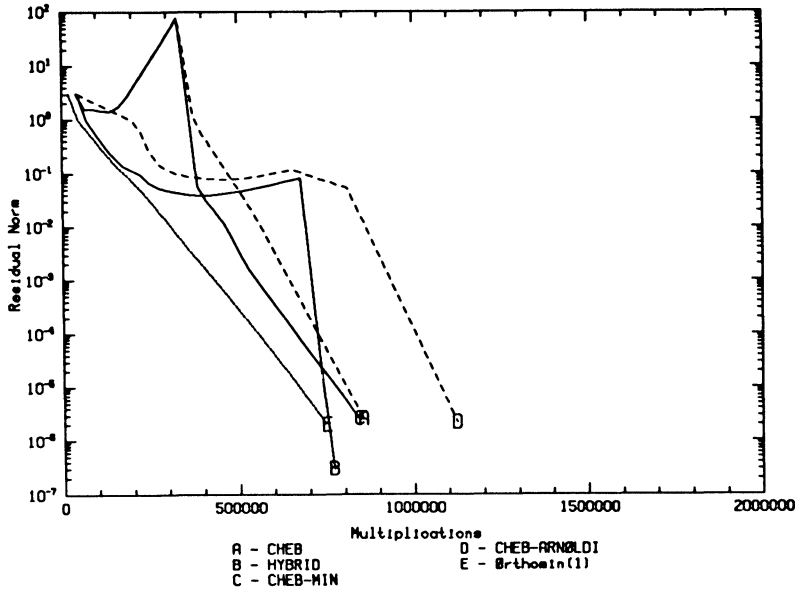

FIG. 5.4. *Problem* 4: $\gamma = 50$, MILU *preconditioning.*

A direct comparison between the two techniques for estimating eigenvalues is somewhat difficult because of the different roles of the growth tolerance parameter τ. In the modified power method, four Chebyshev iterations are performed *after* the condition (25) is violated, so that the residuals will become very rich in the needed eigenvectors. In contrast, Arnoldi's method is performed as soon as (25) is violated, so that the residuals will probably not be dominated as much by these eigenvectors. Without purification, Arnoldi's method (in CHEB-ARNOLDI) does not seem as

effective as the modified power method (in CHEB). However, the combined Arnoldi/GMRES step of HYBRID appears to be more effective than the purified modified power step of CHEB-MIN. It is both less expensive (for $m=4$), and it strongly limits the growth of the residual.

For the third issue, note that inaccurate initial iteration parameters cause the residuals generated by CHEB and CHEB-MIN to diverge by several orders of magnitude in Problems 1, 2 and 4 (the missing eigenvalues take some time to assert themselves in Problem 1). This difficulty is avoided by HYBRID in Problems 1 and 2, where fairly accurate initial eigenvalue estimates combine with the strict growth tolerance $\tau=2$ to prevent divergence. HYBRID does not handle Problem 4 as well. This is because the initial Arnoldi estimates determine a domain of convergence for the Chebyshev iteration that just misses one eigenvalue, and the next Chebyshev iteration diverges too slowly for the adaptive procedure to be invoked until the maximum number of 20 steps is performed. In Problem 3, the eigenvalues are clustered near 1 so that the initial parameters for CHEB and CHEB-MIN are accurate, whereas Arnoldi's method has some difficulty identifying them. The use of Arnoldi's method for initial eigenvalue estimates tends to make the overall performance somewhat smoother, although it may not be necessary if good initial parameters are available.

Finally, note that the performances of Orthomin (1) and the Chebyshev methods are very close. The slopes of the Chebyshev curves are steeper, reflecting their lower cost per step [4], [5], [13], but the overhead of the adaptive steps increases their total cost.

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