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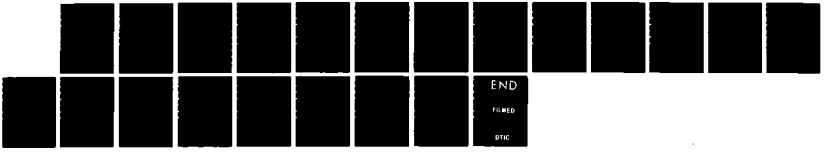

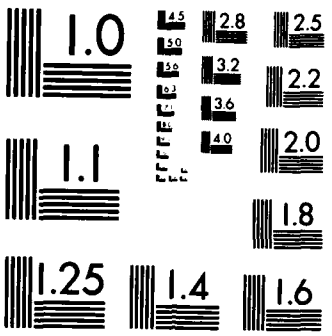

Polynomial Iteration for Nonsymmetric Indefinite Linear Systems

Howard C. Elman[1] and Roy L. Streit[2]

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Abstract

We examine iterative methods for solving sparse nonsymmetric indefinite systems of linear equations. Methods considered include a new adaptive method based on polynomials that satisfy an optimality condition in the Chebyshev norm, the conjugate gradient-like method GMRES, and the conjugate gradient method applied to the normal equations. Numerical experiments on several non-self-adjoint indefinite elliptic boundary value problems suggest that none of these methods is dramatically superior to the others. Their performance in solving moderately difficult problems is satisfactory, but for harder problems their convergence is slow.

1. Introduction

In recent years there has been significant progress in the development of iterative methods for solving sparse real linear systems of the form

$$Au = b, \tag{1.1}$$

where A is a nonsymmetric matrix of order N. One key to this progress has been the derivation of polynomial based methods, i.e. methods whose m-th approximate solution iterate has the form

$$u_m = u_0 + q_{m-1}(A)r_0, \tag{1.2}$$

where u_0 is an initial guess for the solution, $r_0 = b - Au_0$, and q_{m-1} is a real polynomial of degree $m-1$. The residual $r_m = b - Au_m$ satisfies

$$r_m = [I - Aq_{m-1}(A)]r_0 = p_m(A)r_0, \tag{1.3}$$

where p_m is a real polynomial of degree m such that $p_m(0) = 1$. Applying any norm to (1.3) gives

$$\|r_m\| \leq \|p_m(A)\|\|r_0\|.$$

Moreover, if A is diagonalizable as $A = U\Lambda U^{-1}$, then

$$\|p_m(A)\| = \|Up_m(\Lambda)U^{-1}\| \leq \|U\|\|U^{-1}\| \max_{\lambda\in\sigma(A)} |p_m(\lambda)|,$$

so that

$$\|r_m\| \leq \|U\|\|U^{-1}\| \max_{\lambda\in\sigma(A)} |p_m(\lambda)| \, \|r_0\|. \tag{1.4}$$

Thus any polynomial p_m that is sufficiently small on the eigenvalues of A is a good candidate for generating an iterative method.

The conjugate gradient and Chebyshev methods are well-known polynomial-based methods for solving symmetric positive-definite systems for which the residual polynomials $\{p_m\}$ have desirable optimality properties [8]. Generalizations of these techniques have been developed for solving both symmetric indefinite systems (see e.g. [3, 4, 17, 18]), and nonsymmetric systems with definite symmetric part $(A + A^T)/2$ (see e.g. [5, 8, 14] and references therein). In the latter case, all of the eigenvalues of A lie in either the right half or the left half of the complex plane. Sparse linear systems that both are nonsymmetric and have indefinite symmetric part arise in numerous settings. Examples include the discretization of the Helmholtz equations for modelling acoustic phenomena [1] and the discretization of the coupled partial differential equations arising in numerical semiconductor device simulation [12]. Gradient methods that have been proposed as solvers for such problems include the conjugate gradient method applied to the normal equations (CGN) [9], the biconjugate gradient method [7], the restarted generalized minimum residual method (GMRES) [20], and new methods presented in [11, 26]. Smolarski and Saylor [22] and Saad [19] have proposed adaptive polynomial iteration methods of the form (1.2) using polynomials that are optimal with respect a weighted least squares norm. In this paper, we introduce a polynomial-based method, PSUP, that computes a polynomial that is nearly optimal with respect to the Chebyshev norm on a region containing the eigenvalue estimates and then uses this polynomial in (1.2). We compare its performance with the two gradient methods CGN and GMRES.

In Section 2, we give a brief description of the gradient methods CGN and GMRES. In Section 3, we describe the new PSUP method and several heuristics developed to improve its performance. In Section 4, we describe numerical experiments in which these three methods are used to solve some non-self-adjoint indefinite elliptic problems, and in Section 5 we draw conclusions based on the numerical tests.

2. Gradient Methods

In this section we briefly review two conjugate gradient-like methods for solving nonsymmetric indefinite systems. The conjugate gradient method [9] is applicable only to symmetric positive definite linear systems. For nonsymmetric systems, it can be used to solve the normal equations $A^T Ax = A^T b$. The scaled residuals $\{A^T r_m\}$ satisfy

$$A^T r_m = p_m(A^T A) A^T r_0,$$

where p_m is the unique polynomial of degree m such that $p_m(0) = 1$ and $\|r_m\|_2$ is minimum. As is well known, the condition number of $A^T A$ is the square of that of A. Moreover, the standard

implementation of CGN requires two matrix-vector products at each iteration, one by A and one by A^T, plus 5N additional operations. The storage requirement is 4N words. The dependence of CGN on A^TA has led to efforts to find alternatives that are more rapidly convergent and less expensive per step. For nonsymmetric systems with positive definite symmetric part, several methods have been shown to be superior to CGN [5].

GMRES is a method proposed for solving nonsymmetric indefinite systems that avoids the use of the normal equations [20]. Given an initial guess, u_0, for the solution, with residual r_0, this method generates an orthogonal basis $\{v_1, \ldots, v_m\}$ for the Krylov space

$$K_m = \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$$

using Arnoldi's method. Let $v_1 = r_0/\|r_0\|_2$. The Arnoldi process computes for $j = 1, \ldots, m$

$$\begin{aligned} h_{ij} &= (Av_j, v_i), \qquad i = 1, \ldots, j, \\ \hat{v}_{j+1} &= Av_j - \sum_{i=1}^{j} h_{ij} v_i, \\ h_{j+1,j} &= \|\hat{v}_{j+1}\|_2, \\ v_{j+1} &= \hat{v}_{j+1}/h_{j+1,i}. \end{aligned}$$

GMRES then computes an approximate solution

$$u_m = u_0 + \sum_{j=1}^{m} \alpha_j v_j, \tag{2.1}$$

where the scalars $\{\alpha_j\}_{j=1}^m$ are chosen so that $\|r_m\|_2$ is minimum. These scalars can be computed by solving the upper Hessenberg least squares problem

$$\min_{\alpha} \left\| \|r_0\|_2 e_1 - \hat{H}_m \alpha \right\|_2,$$

where $e_1 = (1, 0, \ldots, 0)^T \in \mathbf{R}^{m+1}$ and $\hat{H}_m$ is the Hessenberg matrix of size $(m+1) \times m$ whose (i,j)-entry is h_{ij} [20]. By the choice of basis and the minimization property, $r_m = p_m(A)r_0$ where p_m is the real polynomial of degree m such that $p_m(0) = 1$ and p_m is optimal with respect to the residual norm $\|r_m\|_2$ (c.f. [8] for other formulations of this optimal iteration).

In a practical implementation, the dimension m of the Krylov space is fixed, and the GMRES iteration is restarted with u_m in place of u_0. This is the GMRES(m) method. Defining one "step" to be the average of the m-fold iteration divided by m, the cost per step is $(m + 3 + 1/m)N$ operations plus one matrix-vector product. It requires $(m+2)N$ words of storage.

We remark that the Arnoldi process was originally developed as a technique for computing eigenvalues [27]. Let V_m denote the matrix whose columns are the m vectors generated by the Arnoldi step in GMRES(m), and let H_m denote the square upper Hessenberg matrix consisting of the first m rows of $\hat{H}_m$. Then V_m is an orthonormal matrix of order $N \times m$ that satisfies

$$V_m^T A V_m = H_m. \tag{2.2}$$

Relation (2.2) resembles a similarity transformation, and Arnoldi's method consists of using the eigenvalues of H_m as estimates for (some of) the eigenvalues of A. Suppose $A = U\Lambda U^{-1}$ for diagonal Λ and r_0 is dominated by m eigenvectors $\{u_j\}_{j=1}^m$, with corresponding eigenvalues $\{\lambda_j\}_{j=1}^m$. Then the residual after m GMRES steps satisfies [6]

$$\|r_m\|_2 \leq \|U\|_2 \|U^{-1}\|_2 \; c_m \; \|e\|_2$$

where

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

and e is orthogonal to $\{u_j\}_{j=1}^m$. Loosely speaking, GMRES(m) damps out from the residual the eigenvectors whose eigenvalues are computed by Arnoldi's method.

3. The PSUP Method

The gradient methods just described compute iterates and residuals that satisfy (1.2) and (1.3) (for CGN, with respect to $A^T A$) in which the polynomials are built up recursively without explicit computation of their coefficients. In this section, we describe an alternative iteration that computes explicitly the coefficients of a polynomial $q_{m-1}(z)$ for which $p_m(z) = 1 - zq_{m-1}(z)$ is small on the spectrum $\sigma(A)$. In the following, we will refer to the polynomial $q_{m-1}(z)$ of (1.2) as the "iteration polynomial" and to the polynomial $p_m(z) = 1 - zq_{m-1}(z)$ of (1.3) as the "residual polynomial."

Suppose a compact region $D \subset \mathbf{C}$ contains $\sigma(A)$. Let p_m be a polynomial of degree m that satisfies

$$p_m(0) = 1, \qquad \|p_m\| = \max_{z \in D} |p_m(z)| = \epsilon < 1.$$

As is evident from (1.4), an iteration having p_m as its residual polynomial will result in a decrease of the residual norm if ϵ is small enough. The best possible iteration polynomial with respect to this norm (the Chebyshev norm) is the solution to the minimax problem

$$\epsilon = \min_{q_{m-1}} \max_{z \in D} |1 - zq_{m-1}(z)|. \tag{3.1}$$

Let $q_{m-1}(z) = \sum_{j=0}^{m-1} a_j z^j$. The solution to (3.1) is also the Chebyshev solution to the infinite system of equations

$$\sum_{j=0}^{m-1} z^{j+1} a_j = 1, \qquad z \in \partial D. \tag{3.2}$$

Only the boundary ∂D need be considered because of the maximum modulus principle.

The PSUP method uses an iteration polynomial obtained from an approximate solution to (3.1). We briefly summarize the technique used; details can be found in [24]. First, (3.2) is replaced by a finite dimensional problem

$$\sum_{j=0}^{m-1} z^{j+1} a_j = 1, \qquad z \in \partial D_M, \tag{3.3}$$

where ∂D_M is a finite subset of ∂D containing M points, $M > m$. Equation (3.3) is an overdetermined system of M equations in the m unknowns $\{a_j\}_{j=0}^{m-1}$. The Chebyshev problem for (3.3) is given by

$$\min_{\{a_j\}} \max_{z \in \partial D_M} \Big| \sum_{j=0}^{m-1} z^{j+1} a_j - 1 \Big|. \tag{3.4}$$

Second, equation (3.4) is solved approximately using a semi-infinite linear programming approach to complex approximation, which is based on the identity $|w| = \max_{0 \le \theta < 2\pi} Re(we^{-i\theta})$, $w \in \mathbf{C}$. Let $\Theta = \{\theta_1, \ldots, \theta_p\} \subset [0, 2\pi)$, and define the ***discretized absolute value***

$$|w|_\Theta = \max_{\theta \in \Theta} \; Re(we^{-i\theta}).$$

Consider the discretized problem

$$\min_{\{a_j\}} \max_{z \in \partial D_M} \Big| \sum_{j=0}^{m-1} z^{j+1} a_j - 1 \Big|_\Theta, \tag{3.5}$$

where the absolute value in (3.4) is replaced by the discretized absolute value. This gives rise to a linear program for $\{a_j\}_{j=0}^{m-1}$. Let ϵ^* denote the minimax value of $|\sum_{j=0}^{m-1} z^{j+1} a_j - 1|$ at the solution to (3.4), and let ϵ_p^* denote the minimax value for (3.5). It can be shown that

$$|w|_\Theta \le |w| \le |w|_\Theta \; sec(\alpha/2)$$

for all $w \in \mathbf{C}$, and consequently that

$$\epsilon_p^* \le \epsilon^* \le \epsilon_p^* \; sec(\alpha/2),$$

where α is the smallest difference (mod 2π) between two neighboring angles in Θ. The upper bounds are sharpest for given p when Θ consists of the p-th roots of unity, so that $\alpha = 2\pi/p$. We use this choice of Θ in the following, with $p = 256$ so that $sec(\alpha/2) = 1.000075$.

The dual of the LP (3.5) can be written in the form

$$\min_{S \in \mathbf{R}^{M \times p},\ Q \in \mathbf{R}} Re[e_M^T S e^{-i\Theta}]$$

$$\text{subject to: } S \geq 0, \quad Q \geq 0, \quad Z^T S e^{-i\Theta} = 0 \in \mathbf{C}^m$$

$$\text{and} \quad Q + \sum_{j=1}^{M} \sum_{k=1}^{p} S_{jk} = 1,$$

where $e_M \in \mathbf{C}^M$ is the vector whose components are all 1, $Z \in \mathbf{C}^{M \times m}$ is the coefficient matrix of (3.4), and $e^{-i\Theta} \in \mathbf{C}^p$ denotes the vector whose j-th component is $e^{-i\theta_j}$. Q is a slack variable which must be 0 if $\epsilon_p^* > 0$. A straightforward application of the simplex method to the dual requires $O(Mmp)$ multiplications per simplex iteration and $O(Mmp)$ storage locations. In [24], it is shown that the factor p can be eliminated from these estimates by exploiting the special structure of the dual. These economies leave unaltered the sequence of basic feasible solutions that the simplex method generates en route to the solution. Moreover, they simplify further if the coefficients $\{a_j\}$ are required to be real. In practice the number of simplex iterations has been observed to be $O(m)$ so that the computational effort to compute $\{a_j\}$ using the algorithm in [23] is $O(Mm^2)$. In the experiments discussed below, both M and m are significantly smaller than the order N of the linear system so that construction of the coefficients of the iteration polynomial is a low order cost of the solution process.

Given u_0 and r_0, the basic PSUP iteration consists of repeated application of the iteration polynomial q_{m-1}, as follows:

Algorithm 1: The PSUP iteration.

For $k = 1, 2, \ldots$ Do

$u_{km} = u_{(k-1)m} + q_{m-1}(A) r_{(k-1)m}$

$r_{km} = b - A u_{(k-1)m}$.

The actual computation $w \leftarrow q_{m-1}(A) r$ is performed using Horner's rule:

$w \leftarrow a_{m-1} r$

For $j = 1$ to $m - 1$ Do

$v \leftarrow Aw$

$w \leftarrow a_{m-1-j} r + v$.

The m-fold PSUP iteration requires m matrix-vector products and m scalar vector products, so that the "average" cost is one matrix-vector product and one scalar-vector product. PSUP requires $4N$ storage, for u, r, v and w.

In practice, the PSUP iteration needs estimates of the eigenvalues of A in order to obtain the set D. Several adaptive techniques have been developed for combining an eigenvalue estimation procedure with polynomial iteration [6, 13, 19]. We will use the hybrid technique developed in [6, 19], which uses Arnoldi's method for eigenvalue estimates.

First, the Arnoldi process is used to compute some number k_i of eigenvalue estimates prior to execution of the PSUP iteration. Given these estimates, a set D is constructed that contains them, from which the PSUP iteration polynomial q_{m-1} is computed. (We discuss our choice for D below.) One possible strategy is to perform the PSUP iteration with q_{m-1} until the iteration converges. However, there is no guarantee that all the extreme eigenvalues of A are computed by the Arnoldi procedure. The set D is contained in the lemniscate region [10] $L_m = \{z \in \mathbf{C} \mid |p_m(z)| \leq \epsilon\}$, where ϵ and $p_m = 1 - zq_{m-1}(z)$ solve (3.1). Moreover, the modulus of p_m is greater than ϵ outside L_m and tends to grow rapidly outside L_m, at least in some directions. If an eigenvalue λ lies outside L_m and $|p_m(\lambda)|$ is large enough, then the PSUP method will diverge.

One way to avoid this behavior is to invoke the adaptive procedure: if PSUP diverges then k_a additional Arnoldi steps are performed to compute k_a new eigenvalue estimates. These estimates are then used to construct a new enclosing set D and a new iteration polynomial q_{m-1}, with which the PSUP iteration is resumed. A good choice for a starting vector v_1 is the last residual from the previous PSUP iteration (normalized to have unit norm). For if PSUP diverges, then the residual will tend to be dominated by the eigenvectors whose eigenvalues are not being damped out by the PSUP polynomial. Moreover, this technique can be improved using GMRES. Once the k_a Arnoldi vectors are available, the GMRES(k_a) iteration (2.1) can be performed at relatively little extra expense. This has the effect of damping out from the residual the eigenvector components that were being enhanced by the previous PSUP iteration.

Rather than use the PSUP iteration alone, we consider a hybrid PSUP-GMRES method that makes use of these observations. This method consists of repeated iteration of some number s of PSUP steps, followed by a smaller number k_a of Arnoldi-GMRES steps. The initial eigenvalue estimates are provided by k_i Arnoldi-GMRES steps, where k_i may differ from k_a. In addition, the adaptive procedure is invoked immediately if the residual norm of the PSUP iteration increases

by some tolerance τ relative to the smallest residual previously encountered. The following is a modification of the hybrid method developed in [6] that uses the PSUP iteration:

Algorithm 2: The hybrid GMRES-PSUP method.

Choose u_0. Compute $r_0 = b - Au_0$.

Until Convergence Do

Adaptive (Initialization) Steps: Set v_1 = the current normalized residual,
perform k_a (or k_i) Arnoldi/GMRES steps, and use the new eigenvalue
estimates to update (or initialize) the PSUP coefficients.

PSUP Steps: While $(\|r_j\|_2/\|r_{min}\|_2 \leq \tau))$
Perform s steps of the PSUP iteration (Algorithm 1) to
update the approximate solution u_j and residual r_j.

For the enclosing set D we take the union of the four sets D_j, where D_j is the convex hull of the set of eigenvalue estimates in the j-th quadrant of the complex plane. With this choice, if the extreme eigenvalues of each quadrant have been computed, then all the eigenvalues are contained in D. If all the eigenvalue estimates in either half plane are real, then the part of D containing these estimates is taken to be the line segment between the leftmost and rightmost estimates in the half plane.

There is no guarantee that the eigenvalue estimates computed by Arnoldi's method are accurate. Moreover, since the PSUP residual polynomial has the value 1 at the origin, if D contains points with both positive and negative real parts that are near the origin, then the Chebyshev norm of the residual polynomial will be very close to 1. (See Section 4 for an example.) We consider one heuristic designed to improve the performance of the hybrid PSUP method on problems with eigenvalues very near the origin: we successively remove the points closest to the origin from the set of eigenvalue estimates (and generate a smaller D) until the norm of the PSUP polynomial is smaller than some predetermined value η, and use that polynomial for the PSUP iteration.

There are two possible effects of this heuristic. If the deleted points are not accurate as eigenvalue estimates, then the resulting PSUP iteration will be just as robust and more rapidly convergent than if the deleted points had been included. On the other hand, if the deleted points are good estimates, then the PSUP polynomial will probably be large on the deleted points, and the iteration will not damp out the residual in the direction of the corresponding eigenvectors. However, if the dimension of this eigenspace is small (say, 2 or 3), then the iteration should damp out the residual in all other components, so that the residual should be dominated by a small

number of components. In this situation, a small number of GMRES steps should damp out these dominant components. We will refer to the hybrid PSUP method with this heuristic added as the GMRES/Reduced-PSUP scheme.

We note that with the methods of [24], (3.5) can be also solved with the constraint

$$\max_{z \in E} \left| \sum_{j=0}^{m-1} z^{j+1} a_j - 1 \right|_\Theta \leq 1,$$

where E is some finite set. In particular, if E is the set of deleted eigenvalue estimates in the GMRES/Reduced-PSUP scheme, then the PSUP polynomial on the reduced set D can be forced to be bounded in modulus by one on the deleted points. In experiments with this version of the GMRES/Reduced-PSUP iteration, we found its performance to be essentially the same as that of the unconstrained version described above.

4. Numerical Experiments

In this section, we compare the performance of CGN, GMRES(m), GMRES/PSUP and GMRES/Reduced-PSUP in solving several linear systems arising from a finite difference discretization of the differential equation

$$-\Delta u + 2P_1 u_x + 2P_2 u_y - P_3 u = f, \quad u \in \Omega, \tag{4.1}$$

$$u = g, \quad u \in \partial\Omega,$$

where Ω is the unit square $\{0 \leq x, y \leq 1\}$, and P_1, P_2 and P_3 are positive parameters. We use $f = g \equiv 0$, so that the solution to (4.1) is $u = 0$.

We discretize (4.1) by finite differences on a uniform $n \times n$ grid, using centered differences for the Laplacian and the first derivatives. Let $h = 1/(n+1)$. After scaling by h^2, the matrix equation has the form (1.1) in which the typical equation for the unknown $u_{ij} \approx u(ih, jh)$ is

$$(4-\sigma)u_{ij} - (1+\beta)u_{i-1,j} + (-1+\beta)u_{i+1,j} - (1+\gamma)u_{i,j-1} + (-1+\gamma)u_{i,j+1} = h^2 f_{ij},$$

where $\beta = P_1 h$, $\gamma = P_2 h$, $\sigma = P_3 h^2$ and $f_{ij} = f(ih, jh)$. The eigenvalues of A are given by [21]

$$4 - \sigma + 2\sqrt{1-\beta^2}\cos\frac{s\pi}{n+1} + 2\sqrt{1-\gamma^2}\cos\frac{t\pi}{n+1}, \qquad 1 \leq s, t \leq n.$$

The eigenvalues of the symmetric part are

$$4 - \sigma + 2\cos\frac{s\pi}{n+1} + 2\cos\frac{t\pi}{n+1}, \qquad 1 \leq s, t \leq n.$$

The leftmost eigenvalue of the symmetric part, corresponding to $s = t = n$, is given by

$$(2\pi^2 - P_3)h^2 + O(h^4),$$

so that for small enough h the symmetric part is indefinite when $P_3 > 2\pi^2$.

Six test problems corresponding to six choices of the parameter set $\{P_1, P_2, P_3\}$ are considered. We use the three values $P_3 = 30$, 80, and 250 together with each of the pairs of values $\{P_1 = 1,\ P_2 = 2\}$ and $\{P_1 = 25,\ P_2 = 50\}$. For all tests, $n = 31$, so that the order $N = n^2$ is 969. For all six test problems, the coefficient matrix A is indefinite, and the number of negative eigenvalues of $(A+A^T)/2$ is increasing as P_3 grows. For the first choice of the (P_1, P_2) pair, A is mildly nonsymmetric and its eigenvalues are real, and for the second choice, A is more highly nonsymmetric and has complex eigenvalues.

Although it is not our intention here to examine preconditioners for indefinite systems, preconditioning has been shown to be a critical factor in the performance of iterative methods [3, 5, 15]. In our tests, we precondition (1.1) by the finite difference discretization of the Laplacian. That is, the iterative methods being considered are applied to the *preconditioned problem*

$$AQ^{-1}\hat{x} = b, \quad x = Q^{-1}\hat{x},$$

where Q is the discrete Laplacian. (See [2] for an asymptotic analysis of this preconditioner for finite element discretizations.) The preconditioned matrix-vector product then consists of a preconditioning solve of the form $Q^{-1}v$ and a matrix multiply of the form Av. Since Ω is a square domain, the preconditioning is implemented using the block cyclic reduction method at a cost of $3n^2\log_2 n$ operations [25]. We have confirmed numerically that the preconditioned matrix AQ^{-1} in all six problems has indefinite symmetric part.

We use the following parameters for the hybrid GMRES-PSUP iteration. In an effort to obtain the dominant and subdominant eigenvalues of each quadrant at the outset, the initialization step consists of eight GMRES steps ($k_i = 8$) giving eight eigenvalue estimates. All subsequent calls to the adaptive procedure consist of four GMRES steps ($k_a = 4$). For all tests with PSUP, we use a residual polynomial of degree four ($m = 4$), and allow at most $s = 32$ PSUP steps (or eight successive applications of the PSUP polynomial). The adaptive procedure is invoked if the residual norm increases during a PSUP step ($\tau = 1$), or after s steps are performed. We use $M = 100$ points for the discretized enclosing set ∂D_M, and allocate them so that the number of points in each quadrant is approximately proportional to the circumference of the convex hull in that quadrant. For subsets of D that overlap on quadrant boundaries (e.g. if a line segment on the

real line is shared by regions in the first and fourth quadrants), the shared boundary is discretized twice. For the GMRES/Reduced-PSUP scheme, in which eigenvalue estimates closest to the origin are deleted until the minimax norm is less than some tolerance η, we examine $\eta = .5$ and .3. For this scheme, we take k_a to be two plus the number of eigenvalue estimates deleted. We use the notation GMRES-PSUP(m) (with $m = 4$) for the "unreduced" scheme, and GMRES-PSUP(m, η) for the reduced version.

We examine GMRES(m) for $m = 5$ and $m = 20$. Recall that the latter version generates a higher degree optimal polynomial at the expense of a larger average cost per step.

All numerical tests were run on a VAX 11-780 in double precision (55 bit mantissa). The initial guess in all runs was a vector u_0 of random numbers between -1 and 1. Figures 1 - 6 show the performance of the methods measured in terms of multiplication counts, for the six problems (also numbered 1 - 6). Note that the horizontal scale of Figure 1 is wider than the others, and the scales in Figures 5 and 6 are slightly narrower. Table 1 shows the iteration counts needed to satisfy the stopping criterion of

$$\frac{\|r_j\|_2}{\|r_0\|_2} \leq 10^{-6}.$$

A maximum of 100, 150, and 200 iterations were permitted for the CGN, GMRES and PSUP methods, respectively. (For these iteration counts, CGN, GMRES(20) and GMRES-PSUP(4) performed roughly the same number of operations.) Our main observations on this data are:

1. Problems 1 and 3 are solved efficiently by nearly all the methods, but for the other four problems convergence is slow.

2. In general, the hybrid GMRES-PSUP(m) scheme is weakest. The plateaus in Figures 3, 5 and 6 for this method correspond to the PSUP step, for which convergence is very slow. The "reduction" heuristic improves the performance, but the improvement is due largely to increased effectiveness of the GMRES part of the iteration (e.g. in the steep drops of Figures 2 - 4), and the improved performance is not better than that of GMRES alone.

3. On the whole, GMRES(20) and CGN are the most effective methods for these problems, but they are not dramatically superior to the others. GMRES(20) converges more rapidly than GMRES(5).

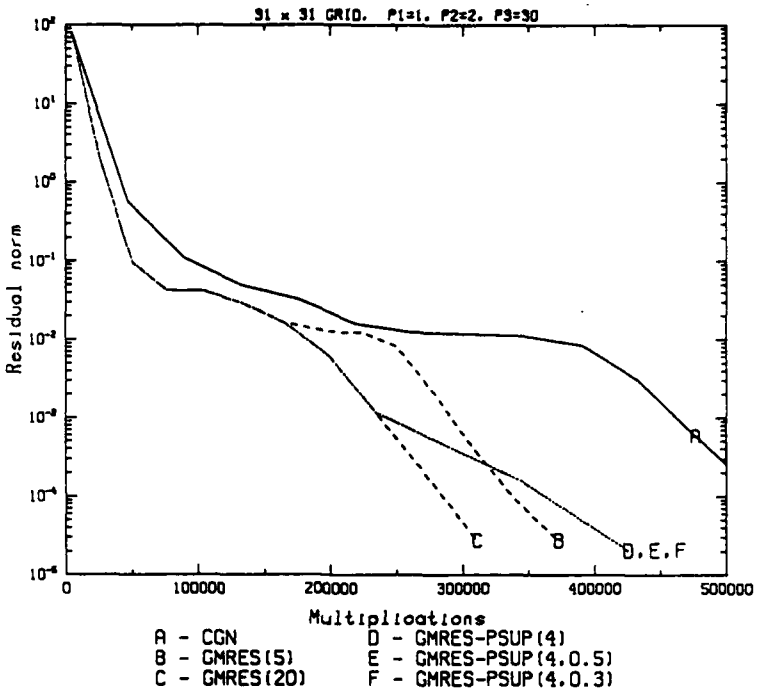

Figure 1: $P_1 = 1$, $P_2 = 2$, $P_3 = 30$

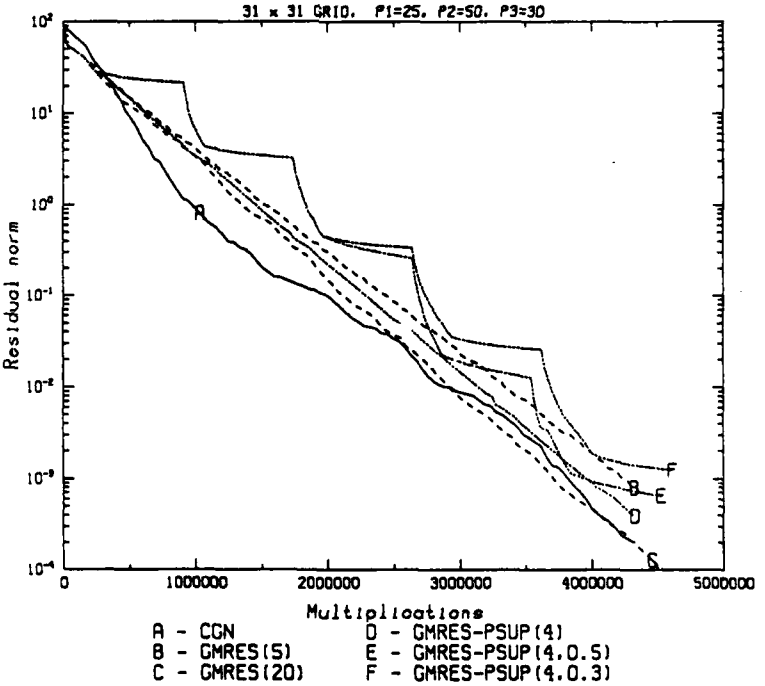

Figure 2: $P_1 = 25$, $P_2 = 50$, $P_3 = 30$

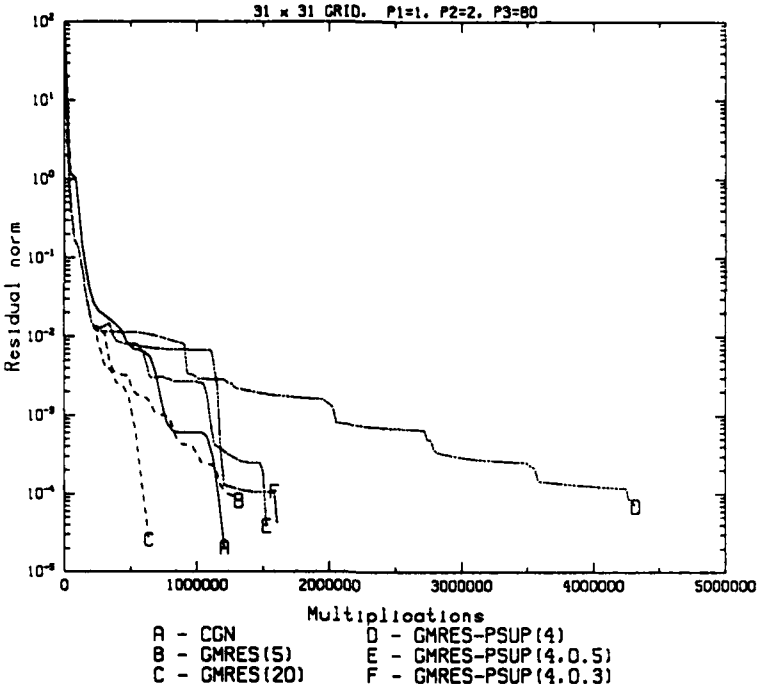

Figure 3: $P_1 = 1$, $P_2 = 2$, $P_3 = 80$

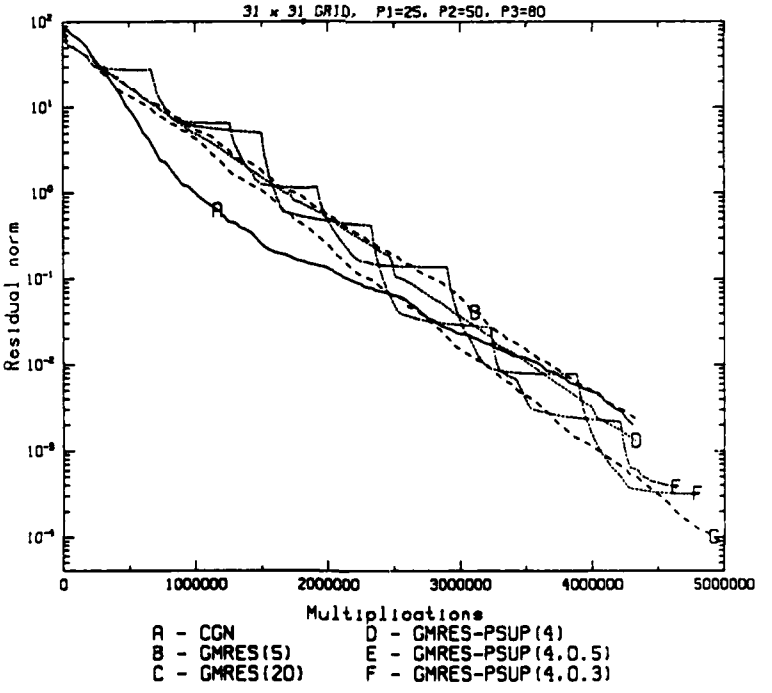

Figure 4: $P_1 = 25$, $P_2 = 50$, $P_3 = 80$

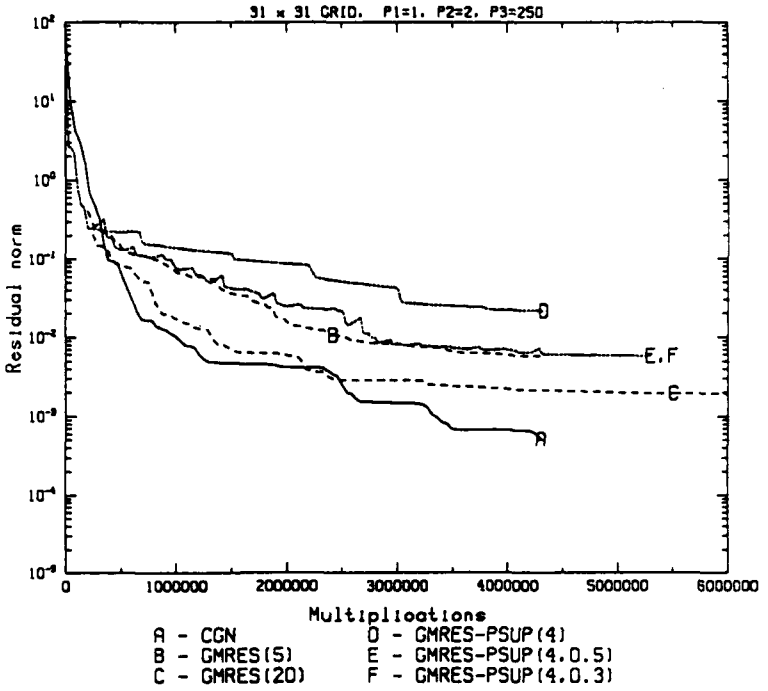

Figure 5: $P_1 = 1$, $P_2 = 2$, $P_3 = 250$

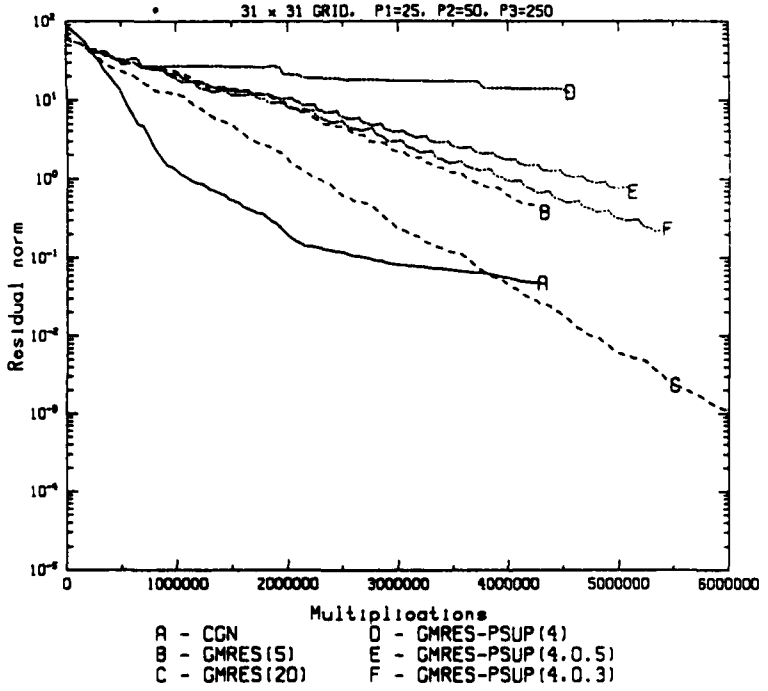

Figure 6: $P_1 = 25$, $P_2 = 50$, $P_3 = 250$

Excluding storage for the matrix and right hand side, the storage requirements for the methods considered are

CGN:	$4N$
GMRES(5):	$7N$
GMRES(20):	$22N$
All PSUP variants:	$10N$

The high cost of the PSUP methods is due to the eight initializing GMRES steps.

Problem #	1	2	3	4	5	6
CGN	13	>100	28	>100	>100	>100
GMRES(5)	13	>150	46	>150	>150	>150
GMRES(20)	10	111	17	119	>150	>150
GMRES-PSUP	16	>200	199	>200	>200	>200
PSUP(4,.5)	16	>200	62	>200	>200	>200
PSUP(4,.3)	16	>200	70	>200	>200	>200

Table 1: Iteration counts.

Although the GMRES/Reduced-PSUP (PSUP(m,η)) scheme is not as fast as pure GMRES, the reduction heuristic does have its intended effect of improving upon the hybrid scheme. We briefly examine the effect of the heuristic on Problem 3, focusing on two curve segments of Figure 3: the plateau of curve D (GMRES-PSUP(4)) between multiplication counts 200000 and 300000, and the last plateau in curve E (GMRES-PSUP(4,.5)). For curve D, on return from the adaptive step at about multiplication count 200000, the real parts of the eigenvalue estimates lie in the intervals [-3,-.33] and [0.4,.98], the Chebyshev norm of the residual polynomial is .98, and convergence is slow. For curve E, on return from the adaptive step prior to the last plateau of the curve, the real parts of the eigenvalue estimates lie in the intervals [-3,-.56] and [.05,.97], and the Chebyshev norm is .96. The effect of deletion of points is shown in Table 2. The Chebyshev norm is very large when there are points near the origin, and it declines as these points are deleted. The deletion of points does not significantly hurt the PSUP part of the iteration and it strongly enhances the effect of the GMRES steps.

We remark that we also considered other variants of the PSUP iteration. In experiments with degrees $m = 6$ and 10 the performance of PSUP was essentially the same.* Moreover, as we noted

*In some tests with degree 16, we were unable to generate the polynomial coefficients. We believe the choice of the powers of z as basis functions makes (3.5) ill conditioned for large m; see [19]. In addition, the implementation based on Horner's rule may suffer from instability for large m.

Deleted Points	Intervals Containing Real Parts	Chebyshev Norm
-	[-3, -.56], [.05,.97]	.96
.05	[-3, -.56], [.34,.97]	.76
.34	[-3, -.56], [.61,.97]	.55
-.56	[-3,-1.46], [.61,.97]	.33

Table 2: Effect of point deletion on GMRES/Reduced-PSUP(4,.5) for Problem 3.

in Section 3, a variant of the GMRES/Reduced-PSUP in which the PSUP polynomial is constrained to be bounded in modulus by one on the set of deleted eigenvalue estimates displayed about the same behavior as the unconstrained version. Similarly, we tested LSQR [16], a stabilized version of CGN, and found that its performance was nearly identical to CGN.

5. Conclusions

The GMRES and PSUP methods are iterative methods that are optimal in the class of polynomial-based methods with respect to the Euclidean or l_∞ norms respectively, for arbitrary nonsingular linear systems. For linear systems in which the coefficient matrix is either symmetric or definite (or both), these types of methods are effective solution techniques [3, 5]. In particular, they are superior to solving the normal equations by the conjugate gradient method. In the results of Section 4, the methods based on polynomials in the coefficient matrix are not dramatically superior to CGN, especially for systems that are both highly nonsymmetric and highly indefinite. GMRES appears to be a more effective method than PSUP.

We note that the best results for other classes of problems depend strongly on preconditioning. We used the discrete Laplacian as a preconditioner in our experiments, and the large iteration/work counts in the results show that this is not a good choice for the given mesh size when the coefficients in the differential operator are large. We believe that improvements in preconditioners are needed to handle this class of problems.

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