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Seymour V. Parter

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Computer Sciences Technical Report #374

January 1980

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Seymour V. Parter[1]

and

Michael Steuerwalt[2]

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†Also to appear as a Los Alamos Scientific Laboratory Report LA-UR-80-263.

[1]Computer Sciences Department, University of Wisconsin-Madison, Madison, WI 53706

[2]University of California, Los Alamos Scientific Laboratory, Los Alamos, NM 87545

*This work was supported by the U.S. Department of Energy under Contract No. W-7405-ENG-36, and by the Office of Naval Research under Contract No. N00014-76-C-0341.

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ABSTRACT

Novel computer architectures and a desire to solve three-dimensional problems have together aroused new interest in iterative methods for computing solutions to elliptic difference equations. Block iterative methods are particularly attractive for vector machines, such as the CRAY-1. Plane iterative schemes reduce a three-dimensional elliptic system to two-dimensional systems. We analyze the convergence rate of k-line and k × k block iterative methods for solving these two-dimensional problems.

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## 1. INTRODUCTION

Some years ago there was great interest in iterative methods for solving elliptic difference equations: see [1, 12, 13, 21, 22, 23, 24]. Recently there has been more emphasis on finite element equations ([2, 4, 5, 20, 25]) and direct methods of solution ([7, 8, 11, 17, 18]). Nevertheless, in practice, particularly in the case of three-dimensional problems (see [9, 11, 19]), finite difference equations are frequently used and they are commonly solved by an iterative method, usually some variant of the SOR method. Furthermore, the advent of new computer architectures, "vector machines" and "parallel processors," has stimulated a search for iterative schemes that are particularly efficient for these machines.

In this report we examine two problems that arise in this way. Consider the three-dimensional model problem

$$(1.1) \qquad -\Delta_h(3)\, U = f \quad , \quad (x_i, y_j, z_n) \in \Omega$$

$$(1.2) \qquad U = g \quad , \quad (x_i, y_j, z_n) \in \partial\Omega$$

where

$$(1.3a) \qquad (x_i, y_j, z_n) = (ih, jh, nh) \quad , \quad 0 \le i,j,n \le P + 1$$

are the grid points in the unit cube $\Omega$ with

$$(1.3b) \qquad h = \frac{1}{P + 1} \quad ,$$

and $\Delta_h(3)$ is the usual 7 point discrete approximation to the Laplace operator, given by

$$(1.4) \qquad \left[\Delta_h(3)U\right]_{ijn} = \begin{cases} \dfrac{U_{i+1,j,n} - 2\,U_{ijn} + U_{i-1,j,n}}{h^2} + \\ \dfrac{U_{i,j+1,n} - 2\,U_{ijn} + U_{i,j-1,n}}{h^2} + \\ \dfrac{U_{i,j,n+1} - 2\,U_{ijn} + U_{i,j,n-1}}{h^2} \end{cases} .$$

Suppose that one has decided to use a "plane" iterative method, probably block SOR where each block is the set of unknowns

$$(1.5) \qquad \tilde{U}_n = \left\{U_{i,j,n} \; ; \; 1 \le i,j \le P\right\}$$

associated with a plane n = constant. Now we must solve the equations in each plane. With $V = \tilde{U}_n$, these equations can be written as

$$(1.6) \qquad 6\,V_{ij} - V_{i+1,j} - V_{i-1,j} - V_{i,j+1} - V_{i,j-1} = F_{ij}, \quad 1 \le i,j \le P \ .$$

We consider two block iterative schemes for the solution of (1.6). These are

(i) k-line iterative scheme: In this scheme each block consists of the unknowns $V_{ij}$ associated with the points on k consecutive horizontal lines. These blocks are indexed by a single index, say s. We have

$$(1.7) \qquad \tilde{V}_s = \left\{ V_{i,k(s-1)+\mu} \ ; \ 1 \le \mu \le k \right\} .$$

(ii) k × k block iterative scheme: In this scheme each block consists of the unknowns $V_{ij}$ associated with the points in a k × k square. It is easiest to describe this block with a double index (r,s). The (r,s) block is

$$(1.8) \qquad \tilde{V}_{rs} = \left\{ V_{k(r-1)+i,k(s-1)+j} \ ; \ 1 \le i,j \le k \right\} .$$

Because each of these block structures satisfies block property A (see [1, 22, 24]) the spectral radii of the Gauss-Seidel method and the SOR method (as well as the optimal overrelaxation parameter $\omega_b$) are determined by the spectral radius of the block Jacobi scheme.

From the analysis of the corresponding block iterative methods applied to the two-dimensional Poisson problem (see [3, 14, 15]), one might expect that these spectral radii behave like 1/k. Unfortunately, this is not the case. In fact, if $\rho(S_k L)$ and $\rho(S_k B)$ are the spectral radii of the block Jacobi iterative methods based on the blocks (1.7) and (1.8) respectively, applied to (1.6), we find that both $\rho(S_k L)$ and $\rho(S_k B)$ have nonzero limits as $k \to \infty$ !

In Section 3 we give the results for the case k = 1. These results are obtained immediately by tensor product methods.

In Section 4 we begin the discussion of our analysis of $\rho(SkL)$ and $\rho(SkB)$. In particular we use a variant of "separation of variables" to reduce the problem to a one-dimensional eigenvalue problem involving tridiagonal matrices.

In Section 5 the basic estimates are obtained. Loosely speaking, we obtain: if $P/k \geq 2$ then

$$\rho(SkL) \to 2 - \sqrt{3} + 0(h^2) = .267949 + 0(h^2) \quad . \tag{1.9}$$

$$\rho(SkB) \to 1/2\ (3 - \sqrt{5}) + 0(h^2) = .381966 + 0(h^2) \quad .$$

Two sets of approximate values for $\rho(SkL)$ and $\rho(SkB)$ are given in the following tables. The results are correct up to a term which is $0(h^2)$.

| k | $\rho_1(SkL)$ | $\rho_2(SkL)$ |
|---|---|---|
| 1 | $1/2 - 3\pi^2h^2/8$ | $1/2 - 3\pi^2h^2/8$ |
| 2 | $1/3 + 0(h)$ | $1/3 + 0(h)$ |
| 3 | .268541 ± .185(-1) | .286398 ± .684(-3) |
| 4 | .267987 ± .483(-2) | .272772 ± .443(-4) |
| 6 | .267949 ± .344(-3) | .268293 ± .221(-6) |
| 8 | .276949 ± .247(-4) | .267974 ± .114(-8) |
| 12 | .267949 ± .127(-6) | .267949 ± .302(-13) |
| 14 | .267949 ± .913(-8) | .267949 |
| 18 | .267949 ± .471(-10) | |
| 24 | .267949 ± .178(-13) | |
| 27 | .267949 | |

Figure 1.

| k | $\rho_1$(SkB) | $\rho_2$(SkB) |
|---|---|---|
| 1 | $2/3 - \pi^2h^2/3$ | $2/3 - \pi^2h^2/3$ |
| 2 | $1/2 + 0(h)$ | $1/2 + 0(h)$ |
| 3 | .384848 ± .515(-1) | .432468 ± .390(-2) |
| 4 | .382296 ± .187(-1) | .400477 ± .477(-2) |
| 6 | .381972 ± .266(-2) | .384625 ± .934(-5) |
| 8 | .381966 ± .387(-3) | .382353 ± .196(-6) |
| 12 | .381966 ± .824(-5) | .381974 ± .888(-10) |
| 14 | .381966 ± .120(-5) | .381967 ± .189(-11) |
| 16 | .381966 ± .175(-6) | .381966 ± .409(-13) |
| 18 | .381966 ± .256(-7) | .381966 |
| 24 | .381966 ± .795(-10) | |
| 30 | .381966 ± .247(-12) | |
| 36 | .381966 | |

Figure 2.

In these tables the shorthand .185(-1) stands for $.185 \times 10^{-1}$. Note that the tolerances for $\rho_2$ are smaller than the tolerances for $\rho_1$, even though the estimates $\rho_1$ appear to converge more rapidly.

As we indicated above, the Jacobi spectral radius determines the spectral radii of the Gauss-Seidel and SOR methods. For the Gauss-Seidel scheme, neglecting $0(h^2)$ terms,

$$\rho(S\infty L\text{-}GS) = \rho(S\infty L)^2 = .071797 \tag{1.10}$$

$$\rho(S\infty B\text{-}GS) = \rho(S\infty B)^2 = .145898 \quad .$$

The optimal $\omega$ for the SOR method is given by

$$\omega_b = 2 \,/\, \left(1 + \sqrt{1-\rho^2}\right)$$

where $\rho$ is the spectral radius of the Jacobi method (see [22]), and with this choice of $\omega$

$$\rho(SOR) = \omega_b - 1 \quad .$$

Hence

$$\begin{aligned} (1.11) \qquad \rho(S\infty L\text{-}SOR) &= .018624 \\ \rho(S\infty B\text{-}SOR) &= .039406 \quad . \end{aligned}$$

Figures 1 and 2 show that in a plane iterative method the inner iterations to solve (1.6) need not use a very large k. Indeed, at k = 8 the spectral radii have essentially reached their asymptotic values.

In Section 6 we describe some computational results. Finally, in Section 7 we comment on the results of this work.

However, one important comment should be made at this point. The analysis given here seems to be very special and possibly limited to model problems. On the other hand, standard elliptic problems can now be handled in great generality by the methods of [3, 13, 15]. Unfortunately, it is not difficult to see that those methods do not, and apparently cannot, apply to these strongly diagonally dominant problems. The elliptic problems discussed in the earlier works are regular problems while the system (1.6) corresponds a two-dimensional discrete singular perturbation problem

$$(1.12) \qquad - h^2 \Delta_h(2)\, U + 2\, U = F \quad .$$

For this reason, and to distinguish from the notation used in [15], we designate the spectral radii as $\rho(SkL)$ and $\rho(SkB)$.

We are indebted to Dan Boley, Bill Buzbee, and Molly Mahaffy for much support and encouragement during the evolution of this work. Bill Buzbee aroused our interest in the problem and provided the basic support, as well as many fruitful discussions. Dan

Boley wrote the original code which was used for experimentation and optimization of the results of [3]. Molly Mahaffy revised Dan Boley's code and carried out the computations described here. These computations were all performed on the CRAY-1 at the Los Alamos Scientific Laboratory.

## 2. Iterative Methods

In this section we describe the basic iterative schemes of interest. Consider a system of linear equations

$$AX = Y \tag{2.1}$$

where A is an R × R matrix. Block iterative schemes for the solution of (2.1) are completely described by describing a partition of the R-vectors into blocks. Specifically, suppose we imagine all R-vectors X partitioned into block vectors of the form

$$X = (X_1, X_2, \ldots, X_{R'})^t \tag{2.2}$$

where each $X_j$ is itself an $R_j$-vector and (of course)

$$\sum_{j=1}^{R'} R_j = R \quad . \tag{2.3}$$

Corresponding to this partition of vectors the matrix A is naturally partitioned into blocks

$$A = A_{ij}$$

where each $A_{ij}$ is itself an $R_i \times R_j$ matrix. In particular, each diagonal block $A_{ii}$ is a square $R_i \times R_i$ matrix. The block Jacobi

iterative scheme associated with this block structure is now given by

$$A_{jj}\, X_j^{(\nu+1)} = -\sum_{j \neq s} A_{js}\, X_s^{(\nu)} + Y_j \quad . \tag{2.4}$$

The corresponding Gauss-Seidel iterative scheme is

$$A_{jj}\, X_j^{(\nu+1)} = -\sum_{j>s} A_{js}\, X_s^{(\nu+1)} - \sum_{j<s} A_{js}\, X_s^{(\nu)} + Y_j \quad , \tag{2.5}$$

while the successive overrelaxation (SOR) iterative scheme with overrelaxation parameter $\omega$ is

$$A_{jj}\, X_j^{(\nu+1)} = -\omega \sum_{j>s} A_{js}\, X_s^{(\nu+1)} - \omega \sum_{j<s} A_{js}\, X_s^{(\nu)} + A_{jj}(1-\omega)\, X_s^{(\nu)} + \omega\, Y_j \quad . \tag{2.6}$$

In every case we have a splitting

$$A = M - N \quad , \tag{2.7}$$

and the iterative scheme takes the form

$$M\, X^{(\nu+1)} = N\, X^{(\nu)} + Y \quad . \tag{2.8}$$

In particular, for the block Jacobi scheme

$$M = \text{diagonal } (A_{ii}). \tag{2.9}$$

For any such splitting, let

$$\rho = \max \left\{ |\lambda| \; ; \; \det(\lambda M - N) = 0 \right\} . \tag{2.10}$$

It is well known ([6, 10, 22]) that if A is nonsingular then the iterates $X^{(\nu)}$ converge to the unique solution X of (2.1) independently of $X^{(0)}$ if and only if

(2.11) $\qquad \rho < 1 \quad .$

Returning to our problem (1.6), we see that our vector X is an R-vector, with $R = P^2$, corresponding to the two-dimensional grid vector $\tilde{U}_n = V$ . Furthermore, (1.7) and 1.8) define two distinct partitions of V.

It is not difficult to see that both partitions lead to Jacobi iterative schemes that satisfy block property A. Hence the Gauss-Seidel spectral radius and the SOR spectral radius, as well as the optimal choice of $\omega$, are determined by the spectral radius $\rho$ of the Jacobi iterative scheme.

The problem studied in this report is: for each of the block Jacobi schemes, k-line and k × k block, determine the asymptotic behavior of $\rho$ as $P \to \infty$ (i.e., as $h \to 0$).

We therefore study the generalized eigenvalue problem

(2.12) $\qquad \lambda M V = N V$

where M is given by (2.9) for the two partitions (1.7), (1.8). In addition to block property A these splittings also have the following properties:

(2.13a) $\qquad M = M^* = M^t$

and M is positive definite;

(2.13b) $\qquad N = N^* = N^t;$

(2.14) $\qquad$ M is an M-matrix -- its inverse $\tilde{M} = (\tilde{M}_{ij})$ satisfies

$$\tilde{M}_{ij} \geq 0 \quad .$$

Finally, $N = (N_{ij})$ also satisfies

(2.15) $$N_{ij} \geq 0 \quad .$$

Other properties of M and N will be developed as needed.

## 3. Estimating $\rho$, $k = 1$

The case $k = 1$ is easily handled by the method of tensor products: see [12, 23]. Here we merely record the results.

Let $\rho(S1L)$ denote the spectral radius of the Jacobi iterative scheme based on a block partition into single lines. Then

(3.1) $$\rho(S1L) = \frac{2 \cos \pi h}{6 - 2 \cos \pi h} \cong \frac{1}{2} (1 - \frac{3}{4} \pi^2 h^2) \quad .$$

Let $\rho(S1^2B)$ denote the spectral radius of the $1 \times 1$ block Jacobi iterative scheme. This is "point" relaxation and we have

(3.2) $$\rho(S1^2B) = \frac{4 \cos \pi h}{6} \cong \frac{2}{3} (1 - \frac{1}{2} \pi^2 h^2) \quad .$$

## 4. Estimating $\rho$, $k \geq 2$. Preliminaries

In this section we develop some general properties of our particular Jacobi iterative schemes. We use these properties to reduce the problems to one-dimensional eigenvalue problems essentially via "separation of variables."

Because our splittings satisfy block property A we know that <u>if</u> $\lambda$ <u>is an eigenvalue of (2.12), so is</u> $-\lambda$ (see [22, 23, 24]). M is positive definite and N is symmetric, so all the eigenvalues of (2.12) are real (see [6]), and thus $\rho$ is characterized by

(4.1) $$\rho = \max_{X \neq 0} \frac{(NX,X)}{(MX,X)}$$

where ( , ) denotes the usual vector inner product

$$(4.2) \qquad (X,Y) = X^t\overline{Y} = \sum x_i \overline{y}_i \quad .$$

Let $k \geq 2$ be a fixed integer less than P. Assume that P is chosen so that k divides P -- that is,

$$(4.3) \qquad P = k\,Q$$

where Q is an integer.

A unified approach to our two problems is provided by the following convenient representation of N in each case. Consider the one-dimensional operator $\tilde{N}$ acting on vectors

$$(4.4) \qquad \phi = (\phi_1, \phi_2, \ldots, \phi_P)^t$$

as follows: for $1 \leq s \leq Q-1$ , $0 \leq j \leq k-1$ ,

$$(4.5) \qquad (\tilde{N}\,\phi)_{ks+j} = \begin{cases} 0 & , \quad 2 \leq j \leq k-1 \\ \phi_{ks+1}, & j = 0 \quad , \\ \phi_{ks} & , \quad j = 1 \quad . \end{cases}$$

Let $N_x$ and $N_y$ be the two-dimensional operators which act on grid vectors $V = (V_{ij})$ in the following manner: $N_x$ acts on V only in the x direction, i.e., the first subscript, and in that direction $N_x$ acts as $\tilde{N}$. Similarly $N_y$ acts on V only in the y direction. For example, for $1 \leq s \leq Q-1$, $0 \leq i \leq k-1$

$$(4.6) \qquad (N_x\,V)_{ks+i,j} = \begin{cases} 0 & , \quad 2 \leq i \leq k-1 \quad , \\ V_{ks+1,j}, & i = 0 \quad , \\ V_{ks,j} & , \quad i = 1 \quad . \end{cases}$$

A careful examination of the two partitions of the matrix A yields the first lemma.

Lemma 4.1: For the k-line Jacobi iterative scheme

$$N = N_y \quad . \tag{4.7a}$$

For the k × k block Jacobi iterative scheme

$$N = N_x + N_y \quad . \tag{4.7b}$$

Lemma 4.2: Let $\rho(SkL)$ and $\rho(SkB)$ be the spectral radii of the k-line and k × k block Jacobi iterative schemes respectively. Then

$$\frac{1}{k+1} + 0(h) \leq \rho(SkL) \leq \frac{1}{3} + 0(h) \quad , \tag{4.8a}$$

$$\frac{2}{k+2} + 0(h) \leq \rho(SkB) \leq \frac{1}{2} + 0(h) \quad . \tag{4.8b}$$

Proof: We first obtain the lower bounds of (4.8). Let $U = (U_{ij})$ be the grid vector

$$U_{ij} = \sin \pi ih \cdot \sin \pi jh \quad . \tag{4.9}$$

Then

$$\frac{(NU,U)}{(MU,U)} = \frac{(NU,U)}{(AU,U) + (NU,U)} \quad .$$

However, U is an eigenvector for A and

$$AU = (4 - 2\cos \pi h)U \cong (2 + 0(h^2))U \quad , \tag{4.10}$$

whence

$$(4.10) \qquad \frac{(NU,U)}{(MU,U)} = \frac{(NU,U)}{(2 + 0(h^2))\ (U,U) + (NU,U)} \quad .$$

A direct calculation using the "smoothness" of U and the form of $\tilde{N}$ (see [3, 14, 15]) shows that

$$(4.11) \qquad (N_x\ U,U) = (2/k + 0(h))\ (U,U)$$
$$(N_y\ U,U) = (2/k + 0(h))\ (U,U) \quad .$$

We put (4.7) and (4.11) into (4.10) and use (4.1) to obtain the lower bounds of (4.8).

Let V be an eigenvector associated with the eigenvalue $\rho$. Then

$$\rho\ M\ V = N\ V \quad .$$

Subtracting $\rho NV$ from both sides gives

$$(4.12a) \qquad A\ V = \mu\ N\ V$$

where

$$(4.12b) \qquad \mu = \frac{1 - \rho}{\rho} \quad .$$

Hence

$$(4.13) \qquad (AV,V) = \mu(NV,V) \quad .$$

It is an easy matter to see, using the explicit eigenvalue of A or the Gerschgorin theorem, that

$$(4.14a) \qquad (AV,V) \geq 2(V,V) \quad .$$

Moreover, the definition of N shows that

$$(4.14b) \qquad (N_y\, V,V) \leq (V,V)$$

$$(4.14c) \qquad \left(\left[N_x + N_y\right]\, V,V\right) \leq 2\ (V,V) \quad .$$

Thus (4.13) and (4.14a), together with (4.14b) or (4.14c), show that $2 \leq \mu$ or $2 \leq 2\mu$, respectively. The upper bounds of (4.8) now follow at once.

Let

$$(4.15) \qquad \sigma = \frac{1}{\mu} \quad .$$

We rewrite (4.12a) as

$$(4.16) \qquad \sigma\, A\, V = N\, V \quad .$$

Any positive eigenvalue $\sigma$ of (4.16) corresponds to a positive eigenvalue $\lambda$ of (2.12) and conversely via the relationships

$$(4.17a) \qquad \sigma = \frac{\lambda}{1 - \lambda}$$

$$(4.17b) \qquad \lambda = \frac{\sigma}{1 + \sigma} \quad .$$

Because $\sigma$ is a monotone increasing function of $\lambda$ (and conversely) we seek the largest positive eigenvalue $\sigma$ of (4.16). But $A^{-1}$ is a positive matrix and $N \neq 0$ is a nonnegative matrix, so by the Perron-Frobenius theory [22] the largest positive eigenvalue of (4.16) is its spectral radius, and the associated eigenvector V may be taken nonnegative.

Let us study the eigenvalue problem (4.16). Because A is positive definite and N is symmetric there is a complete set of eigenvectors $V^{(\nu)}$, $\nu = 1, 2, \ldots, P^2$.

We attempt to apply "separation of variables" to this eigenvalue problem.

Case 1: The k-line scheme.

For each n, $1 \le n \le P$, let

$$V_{ij}^{(n)} = \sin \pi inh \; \phi_j^{(n)} \quad , \qquad 1 \le i,j \le P \quad . \tag{4.18}$$

Substitution into (4.16) with $N = N_y$ yields

$$\sigma A_n \phi^{(n)} = \tilde{N} \phi^{(n)} \quad , \tag{4.19a}$$

where $A_n$ is the tridiagonal matrix

$$A_n = [-1, \; 6 - 2 \cos \pi nh, \; -1] \quad . \tag{4.19b}$$

Each $A_n$ is positive definite, so each eigenvalue problem (4.19a) has P linearly independent eigenvectors, say $\phi^{(n)}(r)$, r = 1, 2, ..., P. Now the vectors given by

$$V_{ij}^{(n)} = \sin \pi inh \; \phi_j^{(n)}(r) \tag{4.20}$$

are $P^2$ linearly independent eigenvectors of (4.16). Hence all the eigenvalues of (4.16) are given by the eigenvalues of the P eigenvalue problems (4.19a), n = 1, 2, ..., P.

We therefore seek the largest positive eigenvalue $\sigma$ of the P eigenvalue problems (4.19a). However, each $A_n$ is not only positive definite but also an M-matrix, i.e., $A_n^{-1}$ is a positive matrix. Because $\tilde{N}$ is a nonnegative matrix, the largest positive eigenvalue of (4.19a) is also the spectral radius of that problem. Moreover, the associated eigenvector $\phi^{(n)}$ may be taken nonnegative. Assume that has been done. Then both V, the eigenvector of (4.16) associated with $\sigma$, and $\phi^{(n)}$, the eigenvector of (4.19a) associated

with $\sigma$, must be nonnegative. Therefore the representation (4.20) shows that we must have

$$n = 1 \quad .$$

We summarize these facts in the following lemma.

Lemma 4.3: Consider the k-line iterative scheme with $2 \leq k < P$ and (4.3) holding. Then

$$\rho(SkL) = \frac{\sigma}{1 + \sigma}$$

where $\sigma$ is the largest positive eigenvalue, and the spectral radius, of the eigenvalue problem

$$\sigma A_1 \phi = \tilde{N} \phi \tag{4.21}$$

and $A_1$ is given by (4.19b) with $n = 1$.

Case 2: The $k \times k$ block scheme.

This case is a bit more complicated, so we proceed with a more formal development of the argument.

Lemma 4.4: Let $N = N_x + N_y$. Consider the eigenvalue problem (4.16) Let $\bar{\sigma}$ be the largest positive eigenvalue. Then $\bar{\sigma}$ is a simple eigenvalue: there is only one linearly independent eigenvector associated with $\bar{\sigma}$. Moreover, the associated eigenvector may be taken to be strictly positive.

Proof: Consider the matrix $A^{-1}N$. Because $A^{-1}$ is a positive matrix and N is a nonnegative matrix not identically zero, every column of $A^{-1}N$ is either the zero vector or a strictly positive vector. Let T be the permutation matrix which collects the positive columns into the first r columns, so that

$$T^t A^{-1} N T = \begin{bmatrix} B_{11} & 0 \\ & \\ B_{21} & 0 \end{bmatrix} = B \quad . \tag{4.22}$$

Here $B_{11}$ is an $r \times r$ positive matrix and $B_{21}$ is a $(P^2 - r) \times r$ positive matrix. Let

$$U = \begin{bmatrix} X \\ Y \end{bmatrix}$$

be an eigenvector of B with associated eigenvalue $\lambda$. Then

$$B_{11} X = \lambda X \quad , \tag{4.23a}$$

$$B_{21} X = \lambda Y \quad . \tag{4.23b}$$

Thus $\lambda$ and X are an eigenvalue and associated eigenvector of $B_{11}$. In particular, if $\lambda = \bar{\sigma}$ then, because $B_{11}$ is strictly positive, there is only one linearly independent eigenvector X and X can be taken strictly positive. Since (4.23b) determines Y uniquely in terms of X, the lemma is proven.

We are now ready to reduce the eigenvalue problem (4.16) to a one-dimensional problem.

Lemma 4.5: Let $N = N_x + N_y$ and consider the eigenvalue problem (4.16). Let $\bar{\sigma}$ be the largest positive eigenvalue. Then $\bar{\sigma}$ is also determined as the largest positive eigenvalue of the eigenvalue problem

$$\sigma B \phi = N \phi \tag{4.24}$$

where

$$\phi = (\phi_1, \phi_2, \ldots, \phi_P)^t \tag{4.25a}$$

and B is the tridiagonal matrix

$$B = [-1, 3, -1] \quad . \tag{4.25b}$$

Proof: The matrix B is both an M-matrix and positive definite. Therefore the eigenvalue problem (4.24) has P linearly independent eigenvectors. Moreover, if $\sigma_0$ is the largest positive eigenvalue the associated eigenvector $\phi^0$ may be taken strictly positive.

Let $\sigma$ be an eigenvalue of (4.24) and let $\phi$ be an associated eigenvector. Let the grid vector V be given by

$$V_{ij} = \phi_i \phi_j \quad . \tag{4.26}$$

Then

$$\sigma(AV)_{ij} = \sigma \phi_i (B\phi)_j + \sigma \phi_j (B\phi)_i \quad .$$

We apply (4.24) to see that

$$\begin{aligned} \sigma(AV)_{ij} &= \phi_i (N\phi)_j + \phi_j (N\phi)_i \\ &= (N_y V)_{ij} + (N_x V)_{ij} = (NV)_{ij} \quad . \end{aligned}$$

In other words, the grid vector V is an eigenvector of (4.16) with associated eigenvalue $\sigma$. In particular, if $\sigma = \sigma_0$ and $\phi = \phi^0$ then the grid vector V is not only an eigenvector of (4.16), it is a strictly positive eigenvector! Hence, by virtue of lemma 4.4, the V so obtained is an eigenvector of (4.16) associated with $\bar{\sigma}$, the largest positive eigenvalue of (4.16). This proves the lemma.

## 5. Estimating $\rho$, $k \geq 3$

In this section we study the one-dimensional eigenvalue problems (4.21), (4.24). We shall first reduce the problem still further by eliminating from (4.21) and (4.24) variables corresponding to those equations in which

$$(\tilde{N}\phi)_j = 0$$

In order to do this we require a specific representation of the solution of tridiagonal systems of equations.

Let $k \geq 3$ be fixed.

Lemma 5.1: Consider the system of linear equations

$$-\phi_{j-1} + \beta\phi_j - \phi_{j+1} = 0 \quad , \qquad j = 1, 2, \ldots, k-2 \tag{5.1a}$$

where $\phi_0$ and $\phi_{k-1}$ are given and

$$\beta > 2 \quad . \tag{5.1b}$$

Let $E_j$, $j = 0, 1, \ldots, k-2$ be generated by the recursive scheme

$$\begin{aligned} E_0 &= 0 \\ E_j &= \frac{1}{\beta - E_{j-1}} \quad , \qquad j = 1, 2, \ldots, k-2, \end{aligned} \tag{5.2}$$

and set

$$\begin{aligned} a_k &= E_1 E_2 \cdots E_{k-2} \quad , \\ b_k &= E_{k-2} \quad . \end{aligned} \tag{5.3}$$

Then

$$\phi_1 = a_k \phi_0 + b_k \phi_{k-1} \quad , \tag{5.4a}$$

$$\phi_{k-2} = b_k \phi_0 + a_k \phi_{k-1} \quad . \tag{5.4b}$$

Furthermore

$$0 < E_j \leq E_{j+1} \leq 1 \quad , \tag{5.5}$$

and as k tends to $\infty$

$$b_k = E_{k-2} \to \frac{1}{2}\left(\beta - \sqrt{\beta^2 - 4}\right), \tag{5.6a}$$

$$a_k \to 0 \quad . \tag{5.6b}$$

Proof: The formulae (5.4a), (5.4b) are obtained from the well known algorithm for solving diagonally dominant tridiagonal systems; see [16, 10]. The monotonicity of the $E_j$ and the bound given in (5.5) are also well known and easily established by induction. Finally, if $k \to \infty$ then $E_{k-2}$ must converge to $E_\infty$, a solution of

$$E^2 - \beta E + 1 = 0 \quad .$$

Because one root is bigger than 1 and the other less than 1, the bound (5.5) implies that $E_\infty$ must be the smaller root. This proves (5.6a). The proof of (5.6b) is immediate from (5.5), (5.6a) and (5.3).

Returning to the eigenvalue problems (4.21) and (4.24), let $1 \le s \le Q-2$ and consider the equations satisfied by $\phi_{ks+2}$, $\phi_{ks+3}$, ..., $\phi_{ks+k-1}$. For the corresponding equations we have $(\tilde{N}\phi)_j = 0$. Hence

$$-\phi_{ks+j-1} + \beta\phi_{ks+j} - \phi_{ks+j+1} = 0 \quad , \quad j = 2, 3, \ldots, k-1 \tag{5.7}$$

where $\phi_{ks+1}$ and $\phi_{k(s+1)}$ can be taken as known. In these equations

$$\beta = 6 - 2\cos \pi h \tag{5.8a}$$

for the eigenvalue problem (4.21) and

$$\beta = 3 \tag{5.8b}$$

for the eigenvalue problem (4.24). In either case we use lemma 5.1 together with the equations numbered ks for s = 2, 3, ..., Q-1 and the equations numbered ks + 1 for s = 1, 2, ..., Q-2 to eliminate $\phi_{ks+j}$, j = 2, 3, ..., k-1 and s = 1, 2, ..., Q-2. For example, the ks equation is

$$\sigma \left[ - \phi_{ks-1} + \beta\phi_{ks} - \phi_{ks+1} \right] = \phi_{ks+1}$$

If $2 \leq s \leq Q-1$, then with the appropriate choice of $a_k$ and $b_k$ we have

$$\phi_{ks-1} = b_k \phi_{ks} + a_k \phi_{k(s-1)+1} \quad .$$

We thus obtain for $2 \leq s \leq Q-1$

$$\sigma \left[ - a_k \phi_{k(s-1)+1} + (\beta - b_k) \phi_{ks} - \phi_{ks+1} \right] = \phi_{ks+1} \quad . \tag{5.9}$$

Similarly, the (ks + 1) equation is

$$\sigma \left[ - \phi_{ks} + \beta \phi_{ks+1} - \phi_{ks+2} \right] = \phi_{ks} \quad .$$

If $1 \leq s \leq Q-2$, then with the appropriate choice of $a_k$ and $b_k$ we have

$$\phi_{ks+2} = a_k \phi_{k(s+1)} + b_k \phi_{ks+1} \quad .$$

Thus we have, for $1 \leq s \leq Q-2$,

$$\sigma \left[ - \phi_{ks} + (\beta - b_k)\phi_{ks+1} - a_k \phi_{k(s+1)} \right] = \phi_{ks} \quad . \tag{5.10}$$

Now we must eliminate $\phi_1$, $\phi_2$, ..., $\phi_{k-1}$ and $\phi_{k(Q-1)+2}$, $\phi_{k(Q-1)+3}$, ..., $\phi_{kQ}$. In these cases we have a system of k - 1 unknowns. However, the procedure is exactly the same. We collect our results in

Lemma 5.2. Let $\sigma \neq 0$ and $\phi$ be an eigenvalue and eigenvector respectively of (4.21) or (4.24). Let $a_k$, $b_k$, and $b_{k+1}$ be given by (5.3) with the appropriate choice of $\beta$, either (5.8a) or (5.8b). Let

$$\xi_{2s-1} = \phi_{ks} \quad , \quad s = 1, 2, \ldots, Q-1 \quad , \tag{5.11a}$$

$$\xi_{2s} = \phi_{ks+1} \quad , \quad s = 1, 2, \ldots, Q-1 \quad . \tag{5.11b}$$

Let

$$\mu = 1/\sigma \quad , \quad \gamma = 1 + \mu \quad . \tag{5.11c}$$

Then $\gamma$ and $\xi_1$, ..., $\xi_{2(Q-1)}$ satisfy the homogeneous system

$$(\beta - b_{k+1})\xi_1 - \gamma\,\xi_2 = 0 \tag{5.12a}$$

$$-\gamma\,\xi_1 + (\beta - b_k)\xi_2 - a_k\,\xi_3 = 0 \tag{5.12b}$$

$$-a_k\,\xi_{2s} + (\beta - b_k)\xi_{2s+1} - \gamma\xi_{2s+2} = 0, \quad s = 1, 2, \ldots, Q-3 \tag{5.12c}$$

$$-\gamma\,\xi_{2s+1} + (\beta - b_k)\xi_{2s+2} - a_k\xi_{2s+3} = 0, \quad s = 1, 2, \ldots, Q-3 \tag{5.12d}$$

$$-a_k\,\xi_{2(Q-2)} + (\beta - b_k)\xi_{2(Q-2)+1} - \gamma\,\xi_{2(Q-1)} = 0 \tag{5.12e}$$

(5.12f) $$- \gamma \xi_{2(Q-2)+1} + (\beta - b_{k+1})\xi_{2(Q-1)} = 0 \quad .$$

Moreover, let $\mu_0$ be the smallest positive number for which the system (5.12) possesses a nontrivial solution; then $\gamma_0 \geq 1$ and

(5.13) $$\rho = \frac{1}{1 + \mu_0} = \frac{1}{\gamma_0} \quad .$$

Proof: It is only necessary to verify the characterization of $\mu_0$ or $\gamma_0$ given by (5.13). However, this is an immediate consequence of our earlier characterization of $\sigma$ as the largest eigenvalue of (4.21) or (4.24).

Corollary: Consider equations (5.12) with $b_{k+1}$ replaced by $b_k$. Let $\hat{\gamma}$ be the smallest positive value $\geq 1$ of $\gamma$ so that these modified equations have a nontrivial solution. Also, consider the system (5.12) with $b_k$ replaced by $b_{k+1}$. Let $\bar{\gamma}$ be the smallest positive value of $\gamma$ so that these modified equations have a nontrivial solution. Then

(5.14) $$\bar{\gamma} \leq \gamma_0 \leq \hat{\gamma} \quad .$$

Proof: Because

$$b_k \leq b_{k+1}$$

we see that

$$\beta - b_{k+1} \leq \beta - b_k \quad .$$

When $\gamma$ is a small positive number the tridiagonal matrix of (5.12) is positive definite. If we increase some diagonal elements (for instance, replace $\beta - b_{k+1}$ by $\beta - b_k$) we increase all the eigen-

values. Thus increasing some diagonal elements means we must raise $\gamma$ to make the system singular. Therefore

$$\gamma_0 \leq \hat{\gamma} \quad .$$

Similarly, replacing $b_k$ by $b_{k+1}$ makes the diagonal smaller and $\gamma$ need not be so large. Thus we have proven (5.14).

Having established this corollary, we proceed to estimate the quantities $\bar{\gamma}$, $\hat{\gamma}$ .

We first rearrange the matrices of interest.

Lemma 5.3: Let $\tilde{A}$ be the symmetric tridiagonal matrix of order $2(Q - 1)$ of the form

$$\tilde{A} = \begin{bmatrix} \bar{\beta} & -\gamma & & & & & \\ -\gamma & \bar{\beta} & -a_k & & & & \\ & -a_k & \bar{\beta} & -\gamma & & & \\ & & -\gamma & \bar{\beta} & -a_k & & \\ & & & & & -\gamma & \\ & & & & -\gamma & \bar{\beta} & \end{bmatrix}$$

That is, the diagonal of $\tilde{A}$ is a constant, $\bar{\beta}$. The superdiagonal is alternately $-\gamma$, $-a_k$, etc.

Let T be the permutation matrix corresponding to the permutation

$$(5.15) \qquad (2j - 1) \to j \quad , \quad 2j \to (Q - 1) + j \quad ,$$

so that, letting $e_j$ denote the $j$th unit vector,

(5.16) $$T = \left[ e_1, e_3, \ldots, e_{2Q-1}, e_2, e_4, \ldots, e_{2(Q-1)} \right] .$$

Then

(5.17a) $$T^t \tilde{A} T = \tilde{B}$$

where

(5.17b) $$\tilde{B} = \begin{bmatrix} \bar{\beta} I & E \\ E^t & \bar{\beta} I \end{bmatrix}$$

and E is the $(Q - 1) \times (Q - 1)$ matrix

(5.17c)

$$\begin{bmatrix} -\gamma & & & \\ -a_k & -\gamma & & \\ & \ddots & \ddots & \\ & & -a_k & -\gamma \end{bmatrix}$$

Proof: Direct computation.

Remark: In the applications of this lemma

$$\bar{\beta} = \beta - b_k \text{ or } \bar{\beta} = \beta - b_{k+1} .$$

Let

(5.18) $$V = \begin{bmatrix} X \\ Y \end{bmatrix}$$

be a nontrivial null vector of $\tilde{B}$, so that

(5.19) $\qquad \tilde{B}\, V = 0 \quad .$

Then (5.19) is equivalent to the pair of equations

(5.20a) $\qquad E^t\, E\, Y = \bar{\beta}^2\, Y \quad ,$

(5.20b) $\qquad E\, E^t\, X = \bar{\beta}^2\, X \quad .$

A computation shows that

(5.21a) $\qquad E^t E =$

$$\begin{bmatrix} a_k^2 + \gamma^2 & a_k\,\gamma & & & \\ a_k\,\gamma & a_k^2 + \gamma^2 & a_k\,\gamma & & \\ & & \ddots & & \\ & & & a_k^2 + \gamma^2 & a_k\,\gamma \\ & & & a_k\gamma & \gamma^2 \end{bmatrix}$$

(5.21b) $\qquad E\, E^t =$

$$\begin{bmatrix} \gamma^2 & a_k\,\gamma & & & \\ a_k\,\gamma & a_k^2 + \gamma^2 & a_k\,\gamma & & \\ & & \ddots & & \\ & & & a_k\,\gamma & \\ & & & a_k\,\gamma & a_k^2 + \gamma^2 \end{bmatrix}$$

That is, $E^tE$ is the constant tridiagonal matrix $[a_k\gamma, a_k^2 + \gamma^2, a_k\gamma]$ except that the $((Q - 1), (Q - 1))$ term is $\gamma^2$ rather than $a_k^2 + \gamma^2$.

Lemma 5.4: Let $\bar{\gamma}$ and $\hat{\gamma}$ be defined as in the corollary to lemma 5.2. Then

$$(5.22) \qquad \begin{aligned} &\beta - b_{k+1} - a_k \le \bar{\gamma} \le \gamma_0 \le \hat{\gamma} \le \\ &\beta - b_k - a_k(1 - 0(h^2)) \le \beta - b_k + a_k \end{aligned}$$

and from (5.13) we have

$$(5.23) \qquad \frac{1}{\beta - b_k + a_k} \le \frac{1}{\beta - b_k - a_k + a_k\, 0(h^2)} \le \rho \le \frac{1}{\beta - b_{k+1} - a_k} \quad .$$

Proof: Consider the case of $\bar{\gamma}$. Then $\bar{\beta} = \beta - b_{k+1}$. From (5.20a) we see that if $\gamma = \bar{\gamma}$ then $\bar{\beta}^2$ is an eigenvalue of $E^tE$. Thus by the Gerschgorin Theorem [6]

$$\bar{\beta}^2 \le a_k^2 + \bar{\gamma}^2 + 2a_k\bar{\gamma} = (a_k + \bar{\gamma})^2 \quad .$$

This establishes the left hand inequality of (5.22).

Consider the case of $\hat{\gamma}$. Then $\bar{\beta} = \beta - b_k$. For $\gamma < \hat{\gamma}$ the matrix $\tilde{B}$ is positive definite. Therefore at $\gamma = \hat{\gamma}$ the smallest eigenvalue of $\tilde{B}$ is zero. Thus $-\bar{\beta}$ is the smallest eigenvalue of

$$\tilde{B}_0 = \begin{bmatrix} 0 & E \\ E^t & 0 \end{bmatrix} .$$

If $\eta$ is an eigenvalue of $\tilde{B}_0$, so is $-\eta$. Moreover, $\eta$ is an eigenvalue of $\tilde{B}_0$ if and only if $\eta^2$ is an eigenvalue of $E^tE$. We

conclude when $\gamma = \hat{\gamma}$ that $\bar{\beta}^2$ is the largest eigenvalue of $E^tE$. Let $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_{Q-1}$ be the eigenvalues of $E^tE$. From the inclusion theorem [6, p. 149] and the known eigenvalues of

$$[\ 1,\ 0,\ 1\ ]$$

we see that

$$\eta_j \geq a_k^2 + \gamma^2 + 2\ a_k\gamma \cos \frac{j\pi}{Q\ -\ 1} \geq \eta_{j+1} \quad , \ 1 \leq j \leq Q-2 \quad .$$

Thus

$$\bar{\beta}^2 \geq a_k^2 + \hat{\gamma}^2 + 2a_k\ \hat{\gamma} \quad \left[1\ -\ \frac{1}{2}\left(\frac{\pi}{Q\ -\ 1}\right)^2\right] \quad .$$

$$\geq a_k^2 + \hat{\gamma}^2 - 2a_k\hat{\gamma} \quad = (\hat{\gamma} - a_k)^2 \quad .$$

It is easy to see that $\hat{\gamma} \leq \bar{\beta}$, whence

$$\bar{\beta}^2 \quad \left[1 + \frac{a_k}{\bar{\beta}} \quad \left(\frac{\pi}{Q\ -\ 1}\right)^2\right] \geq (a_k + \hat{\gamma})^2 \quad .$$

This proves the right hand inequality of (5.22).

Remark: It is important to observe that the coefficient of the $0(h^2)$ term includes $a_k$. Since $a_k \to 0$ rapidly, this term is truly negligible.

Corollary: Let $k \to \infty$ . Then

$$(5.24) \qquad \rho \to \frac{1}{2} \quad \left[\beta\ -\ \sqrt{\beta^2\ -\ 4}\right] \quad .$$

Proof: Using (5.6a) and (5.6b) we see that

$$\rho \to \frac{1}{\beta\ -\ E_\infty} \quad \text{as } k \to \infty \ .$$

However, from the basic equation (5.2) we see that

$$\frac{1}{\beta - E_\infty} = E_\infty = \frac{1}{2}\left[\beta - \sqrt{\beta^2 - 4}\right] .$$

Theorem 5.1: Consider the k-line Jacobi iterative scheme where k divides P and k < P. Let ρ(SkL) denote the spectral radius of this scheme. Then the results shown in Figure 1 are correct up to a term which is $0(h^2)$.

Proof: The result for k = 1 follows from (3.1). The result for k = 2 follows from (4.8a). The results for k ≥ 3 were obtained from a computation based on (5.23) with β = 4. The column $\rho_1$ was computed with the coarse lower bound of (5.23), and $\rho_2$ with the fine lower bound.

Theorem 5.2: Consider the k × k block Jacobi iterative scheme where k divides P and k < P. Let ρ(SkB) denote the spectral radius of this scheme. Then the results shown in Figure 2 are correct.

Proof: The result for k = 1 follows from (3.2). The result for k = 2 follows from (4.8b). The results for k ≥ 3 were obtained from a computation based on (5.23) with β = 3.

## 6. Computational Results

Using codes originally prepared by D. L. Boley (see [3]), Molly Mahaffy computed approximate spectral radii for the Gauss-Seidel iterative scheme using k lines and k × k blocks. These spectral radii were computed by the power method. The Gauss-Seidel method was chosen because the general theory shows that the Jacobi iterative scheme has both ρ and -ρ as eigenvalues while the Gauss-Seidel scheme has a simple eigenvalue on the spectral radius. Furthermore, we also have

$$\rho(\text{Gauss-Seidel}) = \left[\rho(\text{Jacobi})\right]^2 . \tag{6.1}$$

The results are contained in the following tables. In all cases $P = 128$. As with Figures 1 and 2, the columns $\rho_1^2$ and $\rho_2^2$ were computed using the coarser and finer bounds of (5.23), respectively.

k-line Iterative Scheme

| k | $\rho_1^2$ (Theory) | $\rho_2^2$ (Theory) | $\rho^2$ (Computed) |
|---|---|---|---|
| 4 | .071840 ± .259(-2) | .074404 ± .242(-4) | .07662 |
| 8 | .071797 ± .132(-4) | .071810 ± .608(-9) | .07167 |
| 16 | .071797 ± .351(-9) | .071797 | .07164 |
| 32 | .071797 | .071797 | .07164 |
| 64 | .071797 | .071797 | .07164 |

Figure 3.

k × k Block Iterative Scheme

| k | $\rho_1^2$ (Theory) | $\rho_2^2$ (Theory) | $\rho^2$ (Computed) |
|---|---|---|---|
| 4 | .146498 ± .143(-1) | .160382 ± .382(-3) | .16620 |
| 8 | .145898 ± .296(-3) | .146194 ± .150(-6) | .14631 |
| 16 | .145898 ± .134(-6) | .145898 ± .311(-13) | .14590 |
| 32 | .145898 ± .271(-13) | .145898 | .14590 |
| 64 | .145898 | .145898 | .14590 |

Figure 4.

## 7. Comments

It is of interest to observe that the results of Theorem 5.1 and Theorem 5.2 do <u>not</u> require that $k/P \to 0$. In fact, those results are valid as long as $k < P$. This is clearly demonstrated in the computational results. For example, in Figs. 3 and 4 we see that with $P = 128$ and $k = 64$, the largest acceptable value, the value of $\rho^2$ is essentially given by the asymptotic value ($k \to \infty$). These results seem to contradict the intuitive feeling that, were M to include a much larger part of A, the spectral radius would be much smaller.

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