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A LOOK AT TRANSPORT THEORY FROM THE POINT OF VIEW OF LINEAR ALGEBRA

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A LOOK AT TRANSPORT THEORY FROM THE POINT OF VIEW OF LINEAR ALGEBRA

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Abstract. We show that the notion of "preconditioning" from linear algebra can provide a framework for the discussion of algorithms for the numerical solution of the transport equation. In this context we show that the conjugate gradient method yields substantial savings over the Neumann series solution of the standard integral formulation of the transport equation for optically thick regimes. Further, we show that the diffusion synthetic acceleration (DSA) algorithm is the Neumann series solution of the standard integral formulation of the transport equation preconditioned by the Green's function of a diffusion operator. The preconditioned conjugate gradient method, using DSA as a preconditioner, again yields substantial savings.

1 INTRODUCTION

In this paper, we propose to examine the integral equation formulation of the transport equation in slab geometry and the diffusion-synthetic acceleration (DSA) method [La1] for its solution from the point of view of linear algebra. We consider here only the one-dimensional isotropic transport equation, although these ideas can be expanded to the general transport equation.

2 PROBLEM STATEMENT

To fix ideas, the problem we wish to solve is to find $u(1,4)$ given by
where $2a$ represents a measure of the number of mean free paths across the slab. We denote (1) as

\[
\begin{cases}
(\mu D + I)\psi = \gamma L \psi + q \\
B \psi = g(\mu)
\end{cases}
\]

where

\[
D \psi = \frac{\partial\psi}{\partial x}
\]

\[
L \psi = \frac{1}{2} \int_{-1}^{1} \psi(x, \mu')d\mu'
\]

\section{3 INTEGRAL EQUATION FORMULATION}

There exists an invertible operator $H_{\mu}^{-1}$ (the Green's function) such that $H_{\mu}^{-1}q$ is the solution to the differential equation

\[
\begin{cases}
(\mu D + I)\psi = q \\
B \psi = 0
\end{cases}
\]

It is given by

\[
H_{\mu}^{-1} \psi =
\begin{cases}
\frac{1}{\mu} e^{-\mu x} \int_{-a}^{x} e^{\mu s} \psi(s, \mu)ds, & \mu > 0 \\
-\frac{1}{\mu} e^{-\mu x} \int_{x}^{-a} e^{\mu s} \psi(s, \mu)ds, & \mu < 0
\end{cases}
\]

We have $(\mu D + I)H_{\mu}^{-1} = I$, and the solution to

\[
\begin{cases}
(\mu D + I)\psi = q \\
B \psi = g
\end{cases}
\]

is given by $H_{\mu}^{-1}q + \psi_1$, where $\psi_1$ satisfies

\[
\begin{cases}
(\mu D + I)\psi_1 = 0 \\
B \psi_1 = g
\end{cases}
\]
The function $\psi_1$ is given by

$$
\psi_1 = \begin{cases} 
\frac{k_1(\mu)}{\mu} e^{-\mu s}, & \mu > 0, \\
\frac{k_2(\mu)}{\mu} e^{\mu s}, & \mu < 0.
\end{cases}
$$

Thus, the solution to (2) satisfies

$$
\psi = \mathcal{H}_\mu^{-1} \gamma L \psi + \mathcal{H}_\mu^{-1} q + \psi_1.
$$

Operating on (5) by $L$ gives

$$
L\psi = \mathcal{H}_\mu^{-1} \gamma L \psi + q_1,
$$

where the $q_1 = \mathcal{H}_\mu^{-1} q + L \psi_1$ depends only on $\gamma$ and $\mu$. We write this as

$$
(\mathcal{I} - \mathcal{K}) \phi = q_1,
$$

where $\phi = L \psi$ and $\mathcal{K} = \mathcal{H}_\mu^{-1}$. Using (3) we see that

$$
K \phi = \int_{-\mu}^{\mu} k(|x - s|) \phi(s) ds,
$$

where

$$
k(t) = \int_0^\infty \frac{1}{\mu} e^{-\mu t} d\mu.
$$

The properties of $\mathcal{K}$ are well known (cf. [Wi]):

i) $\mathcal{K}$ is self-adjoint, positive definite and compact on $L^2[-\mu, \mu]$.

ii) $\|\mathcal{K}\|_{L^2} < 1$.

iii) $\|\mathcal{K}\|_{L^1} = 1 - O\left(\frac{1}{a^2}\right)$, for large $a$.

iv) If $\sigma_k, u_k$ are an eigenvalue/eigenvector pair of $\mathcal{K}$, then

a) $\sigma_k = O\left(\frac{1}{k}\right)$ for large $k$,

b) $u_k = f_k + O\left(\frac{1}{k}\right)$, where $f_k$ is the $k$th Fourier vector on $[-a, a]$ [FMWW].

4 SPLITTING AND PRECONDITIONING

Let $T$ be any invertible operator, $T\gamma$ - $\mathcal{I}$, and assume that $T\gamma$ is invertible. (We also need $\mathcal{G}$ to operate on the same space as $K$, but we avoid discussion of these mathematical niceties to get on with the story.) We can define a splitting of the operator $T\gamma$ by

$$
T\gamma = (I - K) \gamma + (I - K) \gamma
$$

Equation (7) can now be rewritten as
If we now apply \((I - G\gamma)\), we get the *preconditioned* equation:

\[ (I - G\gamma)^{-1} (I - K\gamma)\phi = q_1 \]  \hspace{1cm} (10)

(Note that this is exactly the equation discussed in [AlWi].) If we had first multiplied \((9)\) by \(T\) and then applied \((T - \gamma I)^{-1}\), we would have gotten the equivalent equation

\[ (I + (T - \gamma I)^{-1} (I -TK)\gamma)\phi = (T - \gamma I)^{-1} Tq_1 = q_2 \]  \hspace{1cm} (12)

The term "preconditioned" arises because we hope to have chosen \(T\) so that the equation \((12)\) is easy to solve, i.e., in some sense "well-conditioned." (Equation \((12)\) is referred to in the DSA algorithm as the "accelerated" equation [Lal].)

## 5 DISCRETIZATION AND ITERATION

Let us discuss for a moment how we would solve an equation like \((7)\) or \((11)\). We start, of course, with a *discretization*. For convenience, we use the same symbol for the discrete operator as the continuous one. The discretization yields a system of linear equations which we solve by using an *iteration* scheme. There are two different questions which arise here. One is the order of accuracy of the discretization (i.e., how close is the solution of the discrete problem to the solution of the continuous problem) and another is the rate of convergence of the iteration scheme (or, more properly, how much work does it take to get an approximate solution within a certain accuracy to the discrete equation). Of course, the two questions are intertwined since we really want an approximate solution within a certain accuracy to the continuous solution. For this analysis we choose to ignore the first question and concentrate on the second.

## 6 NEUMANN SERIES

With this discussion in mind, we note that a standard iteration method for solving the discrete analogue to \((7)\) is

\[ \phi_{n+1} = K\gamma \phi_n + q_1 \]  \hspace{1cm} (13)

Here \(K\) is a discrete operator and \(\phi_n\) and \(q_1\) are discrete vectors. Usually, one does not form the matrix \(K\), but applies \(K\) in the form \(KH_{\mu}^{-1}\); i.e., for a set of \(\mu, j = 1, \ldots, N\), one solves an equation with the operator \(H_{\mu}\), ("invert" \(H_{\mu}\)) and uses a quadrature rule to apply \(f\). The intermediate quantity, \(H_{\mu}^{-1} \gamma \phi_n\), is called \(\psi_n\), the discrete approximation to \(\psi\). The convergence rate of \((14)\) is completely determined by the spectral radius of \(K\gamma\).

Let \(\phi\) be the solution to

\[ \phi = K\gamma \phi + q_1 \]  \hspace{1cm} (14)

and let \(c_n = \phi - \phi_n\). Combining \((13)\) and \((14)\) yields
If the spectral radius of $K\gamma$ is less than 1 (which we write as $\sigma(K\gamma) < 1$), then the iteration will converge. The iteration scheme (13) is perhaps the least sophisticated iterative scheme. Other schemes that have better convergence properties will be discussed later.

The equation (12) can be organized in the same fashion as (13). We write

$$
\phi_{n+1} = (T - \gamma I)^{-1} (TK - I) \gamma \phi_n + q_\gamma
$$

Again, the error equation takes the form

$$
e_{n+1} = (T - \gamma I)^{-1} (TK - I) \gamma e_n = [(T - \gamma I)^{-1} (TK - I) \gamma]^{n+1} e_0
$$

When using (16), we must assume that we have an easy method for applying $T$ and inverting $T - \gamma I$, just as we do for applying $K$. The success of this iteration hinges on the assumption that the spectral radius of $(T - \gamma I)^{-1} (TK - I) \gamma$ is sufficiently less than the spectral radius of $K\gamma$ to justify the extra work involved.

7 BOUNDARY CONDITIONS

There is another point to consider here. When $T$ is a differential operator, for example, it is only invertible when the boundary conditions are considered, that is, when the problem

$$
\begin{aligned}
T u &= f \\
B_T u &= g
\end{aligned}
$$

has a unique solution. Then, we can assume that the Green's function $G$ satisfies

$$
\begin{aligned}
TG - I &= 0 \\
B_T G f &= 0
\end{aligned}
$$

for all $f$.

and the solution to (18) is given by

$$
u = G f + u_1
$$

where

$$
\begin{aligned}
T u_1 &= 0 \\
B_T u_1 &= g
\end{aligned}
$$

In this case, the partial sums for the Neumann series for $\phi$ in (12) are not given uniquely by

$$
(T - \gamma I) \phi_{n+1} = (TK - I) \gamma \phi_n + T q_1
$$

but require boundary conditions to be given on $\phi_{n+1}$. To obtain these boundary conditions, we recall that this scheme was derived from

$$
(I - G \gamma) \phi_{n+1} = (K - G \gamma) \gamma \phi_n + q_1
$$

before we operated on both sides by $T$ (see (10)). If we apply the boundary operator $B_T$ to both sides of (22), we get (since $B_T G = 0$)
so the correct equation for the \((n + 1)\)th partial sum \(Q_{n+1}\) in the iteration (21) is
\[
\begin{align*}
(T - \gamma l) Q_{n+1} &= (TK - l) \gamma Q_n + T q_1 \\
B_T \phi_{n+1} &= B_T K \gamma \phi_n + B_T q_1
\end{align*}
\] (24)

8 EXAMPLE

We include this example to show how DSA falls into this framework. Choose \(T = -\frac{1}{3} D^2 + l\) with boundary equations of the type \(\phi(\pm a) + \beta \phi'(\pm a) = 0\) (see (58)). Then \(G\) is the Green's function for this diffusion operator and the particular boundary conditions chosen. The partial sums of the Neumann series are found from the iteration (24) so that the boundary conditions on \(Q_{n+1}\) are completely determined by the chosen boundary conditions on \(T\). This leads to the scheme
\[
(-\frac{1}{3} D^2 + l - \gamma l) Q_{n+1} = (TK - l) \gamma Q_n + T q_1
\] (25)

Consider the quantity \((TK - l) \gamma Q_n\). Define
\[
\dot{\psi}_n = H_{\mu}^{-1} \gamma \phi_n
\] (26)
or equivalently
\[
H_{\mu} \dot{\psi}_n = \gamma \phi_n
\] (27)
Thus, since \(L \phi_n = \phi_n\), we have
\[
(TK - l) \gamma Q_n = (TLH_{\mu}^{-1} - L) \gamma \phi_n = (TL - LH_{\mu}) \dot{\psi}_n
\] (28)
Now, using the definition of \(T\), we have
\[
TL \dot{\psi}_n = \left(-\frac{1}{3} D^2 + l\right) L \dot{\psi}_n = -\frac{1}{3} D^2 L \dot{\psi}_n + L \dot{\psi}_n
\] (29)
For \(LH_{\mu}\) we get
\[
LH_{\mu} \dot{\psi}_n = L (\mu D + 1) \dot{\psi}_n = DL \mu \dot{\psi}_n + \mu \dot{\psi}_n
\] (30)
(Note that \(DL = LD\) from definitions of \(L\) and \(D\) in (2).) Thus,
\[
(TL - LH_{\mu}) \dot{\psi}_n = \left(-\frac{1}{3} D^2 L \dot{\psi}_n - DL \mu \dot{\psi}_n + D (\frac{1}{3} DL \dot{\psi}_n - L \mu \dot{\psi}_n)
\] (31)
Now operate on (27) by \(L \mu\):
\[
L \mu H_{\mu} \dot{\psi}_n = L \mu \gamma \phi_n
\] (32)
From the definitions of \(L\) and \(\phi_n\) we see that \(\phi_n\) does not depend on \(\mu\). Thus,
\[
L \mu \gamma \phi_n = \gamma \int_1^1 \mu \phi_n (t) \int_1^1 d \mu = 0
\] (33)
Thus,
\[ L\mu H_{\mu} \dot{\psi}_n = DL \mu \dot{\psi}_n + L\mu \ddot{\psi}_n = L\mu (\mu D + I) \dot{\psi}_n = 0. \]  

(34)

or
\[ L\mu \ddot{\psi}_n = -DL \mu \dot{\psi}_n. \]  

(35)

Substituting (35) into (31) yields
\[ (TL - LH_{\mu}) \dot{\psi}_n = D \left( -\frac{1}{3} DL \dot{\psi}_n + DL \mu \dot{\psi}_n \right), \]  

(36)

\[ = \frac{2}{3} D^2 \left( \frac{3\mu^2 - 1}{2} \right) \dot{\psi}_n \]

\[ = \frac{2}{3} D^2 LP_\mu \dot{\psi}_n = \frac{2}{3} D^2 LP_\mu H_{\mu}^{-\frac{1}{2}} \phi_n. \]

where
\[ P_\mu = \frac{3\mu^2 - 1}{2} \]

is the second Legendre polynomial. Thus, the quantity \((TK - I)\phi_n\) necessary for the computation of (25) can be found as the last term in Eq. (36). This agrees exactly with the DSA algorithm as described in [La1].

9 OTHER ITERATION SCHEMES

It is not necessary to solve Eq. (7) by the Neumann series iteration (13), nor is it necessary to solve the preconditioned Eq. (12) by the iteration (16). In this section, we will describe several iterative methods for solving (7) or (12). Consider a general linear system
\[ Ax = b. \]  

(37)

If \(x_0\) is an initial guess at the solution, we let
\[ r_0 = b - Ax_0 \]  

(38)

be the initial residual. A class of iterative schemes called gradient or polynomial methods is characterized by choosing \(x_{i+1}\) to be \(v_i\) plus some linear combination of previous residuals, that is,
\[ x_{i+1} = v_i + \sum_{j=0}^{i} \alpha_{ij} r_j. \]  

(39)

If \(e_i = v_i - v_i\) is the error, it is easy to see that (cf. [FaMa])
\[ e_{i+1} = p_{i+1}^i(A) e_0, \]  

(40)

where \(p_{i+1}^i(\lambda)\) is a polynomial of degree \(i + 1\) such that \(p_{i+1}(0) = 1\). The convergence properties of such schemes depend upon choosing \(p_{i+1}(\lambda)\) to be small on all of the eigenvalues of \(A\).
Of course, it is not economical to keep all of the previous residuals. Three such algorithms that require only two auxiliary vectors are the nonstationary one-step method, or Richardson's iteration; a nonstationary two-step method known as the Chebyshev iteration; and the conjugate gradient iteration. We will describe first the Richardson's iteration and show that the Neumann series is perhaps the simplest such algorithm. If we let

\[ x_{i+1} = x_i + \alpha_i r_i, \]

then

\[ e_{i+1} = e_i - \alpha_i r_i = (I - \alpha_i A) e_i, \]

or

\[ e_{i+1} = \prod_{j=0}^{i} (I - \alpha_j A) e_0. \]  

Thus, the polynomial is given by

\[ p_{i+1}(\lambda) = \prod_{j=0}^{i} (1 - \alpha_j \lambda), \]

and the roots of \( p_{i+1}(\lambda) \) are \( \frac{1}{\alpha_j}, j = 0, \ldots, i \). If the eigenvalues of \( A \) lie on some interval on the positive real axis, then the roots of \( p_{i+1}(\lambda) \) might be chosen so that \( p_{i+1}(\lambda) \) is the scaled and translated Chebyshev polynomial on the interval. This polynomial has a minimax property that makes it "as-small as-possible" on the interval (cf. [GoVa]).

Now consider Eq. (13). Here \( A = (I - K\gamma) \). If we rearrange the terms we have

\[ \phi_{n+1} = \phi_n + (q_1 - (I - K\gamma)\phi_n) = \phi_n + r_n. \]

The corresponding error equation is

\[ e_{n+1} = (I - A)e_n = (I - A)^{n+1}e_0. \]

Thus, the iteration (13) is a Richardson iteration with \( \alpha_i = 1 \). The polynomial \( p_i(\lambda) \) has all of its roots at 1.0. It is well known that \( K\gamma \) is symmetric positive definite and \( \|K\gamma\| < 1 \). Thus, the eigenvalues of \( A = (I - K\gamma) \) lie in some interval \([\varepsilon, 1.0]\), where \( \varepsilon = 1 - \|K\gamma\| \). The convergence factor for the iteration (13) is

\[ \|e_{i+1}\| \leq \|K\gamma\|^{i+1} \|e_0\| = (1 - \varepsilon)^{i+1} \|e_0\|. \]

The convergence factor for choosing the scaled and translated Chebyshev polynomial would be

\[ \|e_{i+1}\| \leq 2 \left( \frac{1 - \sqrt[2i]{\varepsilon}}{1 + \sqrt[2i]{\varepsilon}} \right) \|e_0\| \]

(cf. [GoVa]).

The iteration (41) with the \( \alpha_i \)'s chosen to be the reciprocals of the roots of the \( i+1^{st} \) scaled and translated Chebyshev polynomial will only yield the Chebyshev polynomial in
(43) on the $i+1$th step. Because of certain recursion properties of the Chebychev polynomials, it is possible to design an algorithm of the form

$$r_i = b - Ax_i \quad (48a)$$

$$\Delta_i = \alpha_i r_i + \beta_i \Delta_{i-1} \quad (48b)$$

$$x_{i+1} = x_i + \Delta_i \quad (48c)$$

where the $\alpha_i$'s and $\beta_i$'s are chosen so that at every step $p_j(\lambda)$ is the $j$th scaled and translated Chebychev polynomial. All that is needed is to know the interval on the real axis that contains the eigenvalues. This can be done dynamically using estimates made available during the iteration. We also mention that this iteration may be applied to certain linear systems with complex eigenvalues (cf. [Ma1],[Ma2]).

The conjugate gradient iteration (CG) (cf. [HeSt],[Re]) can be applied to (37) if, as in our case, the matrix $A$ is symmetric positive definite. The iteration is of the form

$$x_{i+1} = x_i + \alpha_i p_i , \quad \alpha_i = \frac{<r_i,r_i>}{<Ap_i,p_i>} \quad (49a)$$

$$r_{i+1} = r_i - \alpha_i Ap_i \quad (49b)$$

$$p_{i+1} = r_{i+1} + \beta_i p_i , \quad \beta_i = \frac{<r_{i+1},r_{i+1}>}{<r_i,r_i>} \quad (49c)$$

where $<\cdot,\cdot>$ represents vector inner product. Like all of the iterations in this class, the error equation is of the form (40). Now, however, the polynomial $p_{i+1}(\lambda)$ is chosen so that $e_{i+1}$ is optimal at each step in a certain norm. Therefore, the conjugate gradient iteration is at least as good as the Chebychev iteration if the error is measured in this norm.

Let us compare the convergence of the Neumann series with that of a Chebychev or conjugate gradient iteration for an optically thick slab, that is, for large $a$. Since $\|K\|_{L_1} = 1 - 0 \left(\frac{1}{a^2}\right)$, [Wi], we can replace $\varepsilon$ in (46) and (47) by $\left(\frac{k_0}{a}\right)^2$, where $k_0$ is a constant with respect to $a$. We may ask how many steps of the Neumann series (46) yield the same error reduction as one step of a CG iteration (47). In other words, we seek $m$ such that

$$\left(1 - \frac{k_0}{a}\right)^m = \left[1 - \frac{k_0}{a}\right] \left[1 + \frac{k_0}{a}\right]$$

for large $a$. Taking the log of both sides and expanding we find that

$$m = \frac{2a}{k_0} + O\left(\frac{1}{a}\right) \quad (50)$$
For example, if \( a = 128 \), then \( \epsilon = 5.36 \times 10^{-5} \) and \( m = 273 \). That is, each iteration of the Chebychev on conjugate gradient method is equivalent to approximately 273 iterations of the Neumann series. In practice, \( CG \) often performs even better. This is due to the fact that the \( CG \) iteration can take advantage of the distribution of eigenvalues in the interval containing the spectrum (cf. \([\text{HeSt}]\)).

Another advantage of the \( CG \) iteration is that very good estimates of the extreme eigenvalues can be calculated at little cost from the iteration parameters (\([\text{GoVL}]\)). Thus, \( \|K\| \) can easily be approximated. Similar approximation can be calculated from the Chebychev iteration (\([\text{Ma2}]\)).

10 PRECONDITIONED ITERATIVE SCHEMES

It is possible to combine a splitting or preconditioning with the iterative methods discussed in the previous section. The general idea is to multiply the equation (37) by a matrix \( C \) to yield the new system

\[
CAx = Cb
\]

with hopefully better properties than the original system. Equation (41) becomes

\[
x_{i+1} = x_i + \alpha_i Cr_i
\]

which yields

\[
e_{i+1} = p_{i+1}(CA)e_0
\]

Likewise, \( r_i \) can be replaced by \( Cr_i \) in (48b) to yield a preconditioned Chebychev iteration.

Now, it is the spectral properties of \( CA \) that become important. If the eigenvalues of \( CA \) lie in the right-half plane, parameters \( \alpha_i \) and \( \beta_i \) can be chosen so that the preconditioned Chebychev iteration converges (\([\text{Ma1}]\)).

In the context of this paper, we have \( A = I - Ky \) and \( C = (I - G \gamma)^{-1} \). As in (11) we have

\[
CA = (I - G \gamma)^{-1}(I - K \gamma) = (I - (I - G \gamma)^{-1}(K - G \gamma)).
\]

Since both \( A \) and \( C \) are symmetric and positive definite, the spectrum of \( CA \) is positive and real. In this case, a preconditioned conjugate gradient iteration may be employed (cf. \([\text{CGO}]\)):

\[
x_{i+1} = x_i + \alpha_i p_i \quad \alpha_i = \frac{<Cr_i, r_i>}{<Ap_i, p_i>},
\]

\[
r_{i+1} = r_i - \alpha_i Ap_i
\]

\[
P_{i+1} = \beta_i p_i \quad \beta_i = \frac{<r_{i+1}, r_{i+1}>}{<r_i, r_i>}
\]

Convergence rates for both Chebychev and preconditioned conjugate gradients are given by
where

\[ c = \text{Cond}_A(CA) = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} \]  \hspace{1cm} (57)

and \( \lambda_{\text{max}} \) and \( \lambda_{\text{min}} \) are the maximum and minimum eigenvalues of \( CA \), respectively.

In particular, the conjugate gradient iteration can be used in conjunction with the DSA preconditioning. Before we examine this numerically, let us first derive a better understanding of the properties of the DSA preconditioning.

11 PROPERTIES OF THE DSA PRECONDITIONING

In this section, we illustrate the properties of the DSA splitting that make it a good preconditioning. Our point of take-off here is the example in Section 8. We focus on the case \( y = 1 \), since it is the most difficult problem to solve. Let

\[
\begin{align*}
T_\beta \phi &= (-\frac{1}{3}D^2 + I)\phi \\
B_\beta \phi &= \phi(\pm a) + \beta \phi'(\pm a) = 0.
\end{align*}
\]  \hspace{1cm} (58)

The eigenvectors of \( T_\beta \) will be of the form

\[ v_k(x) = a_k \cos \left( \frac{\eta_k x}{a} \right) + b_k \sin \left( \frac{\eta_k x}{a} \right). \]  \hspace{1cm} (59)

Substituting (59) into (58) yields

\[ \frac{\beta}{a} \eta_k = -\tan (\eta_k). \]  \hspace{1cm} (60a)

or

\[ \frac{\beta}{a} \eta_k = \cot (\eta_k). \]  \hspace{1cm} (60b)

In Fig. 1 the graphs \( y = \frac{\beta}{a} \eta \), \( y = -\tan (\eta) \), and \( y = \cot (\eta) \) are plotted. The intersections are values of \( \eta_k \). Notice that for \( \beta > 0 \)

\[ \eta_k \in \left( k - \frac{1}{2}, k + \frac{1}{2} \right). \]  \hspace{1cm} (61)

and for \( \frac{\beta k}{a} \ll 1 \)

\[ \eta_k = \frac{k \pi}{2} + \frac{\beta k \pi}{2a} + O \left( \left( \frac{\beta k}{a} \right)^2 \right). \]  \hspace{1cm} (62a)
while for $\beta_k a \gg 1$

$$\eta_k = (k - 1) \frac{\pi}{2} + \frac{2a}{\beta_k \pi} - O \left( \left\{ \frac{a}{\beta_k} \right\}^3 \right).$$

(62b)

The values $\eta_k$ migrate from the right end of $((k - 1) \frac{\pi}{2}, k \frac{\pi}{2})$ to the left. Putting this all together we see that the eigenvectors of $T_\beta$ are

$$v_k = \begin{cases} 
\cos \left( \frac{\eta_k}{a} x \right), & \text{for } k \text{ odd} \\
\sin \left( \frac{\eta_k}{a} x \right), & \text{for } k \text{ even}
\end{cases}$$

(63)

Finally, if $G_\beta$ is the Green's function for $T_\beta$, the eigenvalues of $G_\beta$ are given by

$$\lambda_k = \frac{1}{1 + \frac{1}{3} \left( \frac{\eta_k}{a} \right)^2}$$

(64)

For $\beta_k a \ll 1$ we have

$$\lambda_k = \frac{1}{1 + \frac{1}{3} \left( \frac{k \pi}{2a} \right)^2}$$

(65)
The parameter $\beta$ can be used to control the shape of the eigenvectors of $G_\beta$ near the boundary of the slab. Figure 2 displays the condition of $CA = (I - G_\beta)^{-1}(I - K)$ as a function of $\beta$ for $a = 1$. The $\beta$ for which the condition is minimized will yield the best preconditioning (cf. (56)). Notice that the condition is approximately $1.25$ over a wide range of $\beta$'s near the value of $\beta = \frac{2}{3}$. This agrees with the results found in [La1]. In fact, the condition takes on the value $1.240276$ for values of $\beta$ in the interval $(.68, .76)$.

For very large $a$, the value of $\beta$ in the range $[0,1]$ has little impact on the largest eigenvalues of $G_\beta$ (cf. (62a)). The corresponding eigenvectors of $G_\beta$ also closely match those of $K$. Let us now examine the operator $K$.

12 THE OPERATOR $K$

First consider $H_\mu$. A singular value/vector decomposition of $H_\mu$ yields

$$H_\mu^{-1}f = \sum_{k=1}^\infty \frac{\delta_0(\zeta_k)}{a \delta_0(\zeta_k)} \begin{cases} \int_{-a}^a \sin \left( \frac{x+\mu}{2a} \right) \sin \left( \frac{x-\mu}{2a} \right) f(s)ds, \mu > 0, \\ \int_{-a}^a \sin \left( \frac{x-\mu}{2a} \right) \sin \left( \frac{x+\mu}{2a} \right) f(s)ds, \mu < 0, \end{cases}$$

(66a)

where

$$a \delta_0(\zeta_k) = a \left[ 1 - \frac{\sin \left( \frac{2\zeta_k}{\zeta_k} \right)}{2\zeta_k} \right] = \int_{-a}^a \sin^2 \left( \frac{x+\mu}{2a} \right) dx$$

(66b)
is a normalization factor. The values \( \zeta_k \) are the positive roots of the equation

\[
\frac{|\mu|}{2a} \zeta = -\tan (\zeta). \tag{67}
\]

The roots of (67) are very similar to the roots of (60a,b). Now, however, for \( \frac{\mu k}{2a} \ll 1 \)

\[
\zeta_k = k \pi - \frac{\mu k}{2a} + \frac{1}{2} \left( \frac{\mu k}{2a} \right)^2.	ag{68a}
\]

while for \( \frac{\mu k}{2a} \gg 1 \),

\[
\zeta_k = \left( k - \frac{1}{2} \right) \pi + \frac{2a}{\mu k} - \frac{1}{2} \left( \frac{2a}{\mu k} \right)^2.\tag{68b}
\]

To find \( K \) we must apply \( L \) to (66a). Applying \( L \) to a single term of (66a) yields

\[
\left\{ \frac{1}{2} \int_0^1 \frac{\cos (\zeta_{k} \mu)}{a \delta_0 (\zeta_{k})} \sin \left[ \frac{\zeta_k}{2} \frac{x + a}{2a} \right] \sin \left[ \frac{\zeta_k}{2} \frac{x - a}{2a} \right] d\mu \right. \\
\left. + \frac{1}{2} \int_{-1}^0 \cos (\zeta_{k} \mu) \sin \left[ \frac{\zeta_k}{2} \frac{x + a}{2a} \right] \sin \left[ \frac{\zeta_k}{2} \frac{x - a}{2a} \right] d\mu \right\}. \tag{69}
\]

Since \( \zeta_k (\mu) = \zeta_k (-\mu) \) we can combine the two integrals above. Expanding each \( \sin \) term and combining yields

\[
\left\{ \frac{1}{2} \cos (\zeta_{k} \mu) \cos \left[ \frac{\zeta_k}{2} \frac{x}{a} \right] \cos \left[ \frac{\zeta_k}{2} \frac{s}{a} \right] \\
- \sin^2 \left[ \frac{\zeta_k}{2} \frac{x}{a} \right] \cos \left[ \frac{\zeta_k}{2} \frac{s}{a} \right] \cos \left[ \frac{\zeta_k}{2} \frac{s}{a} \right] \right\} d\mu. \tag{70}
\]

While (70) does not constitute a singular value/vector decomposition of \( K \), it does yield useful bounds for large \( a \) (since \( K \) is self-adjoint and positive definite, its singular vector/value decomposition is also its eigenvalue/vector decomposition). First, notice that for \( \mu \neq 0 \) as \( k \) increases, \( \zeta_k \) migrates from \( k \pi \) to \( (k - \frac{1}{2}) \pi \) and consequently \( \cos (\zeta_{k} \mu) \) migrates from 1 to 0. Using (68b), we see the terms decrease like

\[
|\cos (k - \frac{1}{2}) \pi + \frac{2a}{\mu k} | \sin \left( \frac{2a}{\mu k} \pi \right) \approx \frac{2a}{\mu k} \approx 1.
\]

Now try \( \mu \). Notice that \( \sin \left( \frac{\zeta_k}{2} \frac{x}{a} \right) \) is odd while \( \cos \left( \frac{\zeta_k}{2} \frac{y}{a} \right) \) is even, and thus they are orthogonal in \( \int_{[-a,a]} d\mu |d\mu| \). Each term of (70) is a self-adjoint rank two operator, \( R_k (\mu) \), already decomposed into its eigenvector expansion. For \( \frac{k}{a} \ll 1 \), one eigenvalue is close to 1 and the other is close to zero. Also, for \( \frac{k}{a} \gg 1 \), the operators \( R_k (\mu) \) are nearly mutually
orthogonal. Since the integration with respect to \( \mu \) involves a very small range of \( \xi \), the integrated terms retain these properties.

For \( \frac{k}{d} \) not small, \( \xi \) is no longer close to \( k\pi \) and thus, the \( R_{k}(\mu) \) are no longer mutually orthogonal. Moreover, the integration with respect to \( \mu \) involves a larger interval of \( \xi \). The behavior is no longer clear. However, large \( k \) denotes high frequency. Notice that

\[
\frac{1}{d} \int_{-a}^{a} \sin \left( \frac{\xi_k}{2} \frac{x}{d} \right) \sin \left( \frac{\xi_l}{2} \frac{x}{d} \right) dx = 2 \left[ \frac{\sin \left( \frac{\xi_k - \xi_l}{2} \right)}{(\xi_k - \xi_l)} - \frac{\sin \left( \frac{\xi_k + \xi_l}{2} \right)}{(\xi_k + \xi_l)} \right]
\]

\( (71a) \)

\[
\approx \frac{1}{|\xi_k - \xi_l|}.
\]

Likewise,

\[
\frac{1}{d} \int_{-a}^{a} \cos \left( \frac{\xi_k}{2} \frac{x}{d} \right) \cos \left( \frac{\xi_l}{2} \frac{x}{d} \right) dx = 2 \left[ \frac{\sin \left( \frac{\xi_k - \xi_l}{2} \right)}{(\xi_k - \xi_l)} + \frac{\sin \left( \frac{\xi_k + \xi_l}{2} \right)}{(\xi_k + \xi_l)} \right]
\]

\( (71b) \)

is of the same order. While not mutually orthogonal the high-frequency terms are nearly orthogonal to the low-frequency terms. Often \( \frac{k}{d} \ll 1 \), for frequencies of interest. Now we will examine the behavior of the largest eigenvalues of \( K \) for \( \frac{k}{2a} \ll 1 \). First let \( \xi_k = k\pi - \theta_k \). We have

\[
0 \leq \theta_k \leq \frac{1}{2} \frac{mk\pi}{2a}.
\]

\( (72) \)

Notice that

\[
\cos^2 \left( \frac{\xi_k}{2} \right) = \frac{1}{2} \left( 1 + (-1)^k \cos (\theta_k) \right)
\]

\( (73a) \)

\[
\sin^2 \left( \frac{\xi_k}{2} \right) = \frac{1}{2} \left( 1 - (-1)^k \cos (\theta_k) \right)
\]

\( (73b) \)

Thus, the odd terms of \( (70) \) are dominated by \( \cos \left( \frac{\xi_k}{2} \right) \cos \left( \frac{\xi_k}{2} \right) \), while the even terms are dominated by \( \sin \left( \frac{\xi_k}{2} \right) \sin \left( \frac{\xi_k}{2} \right) \). Compare this with the eigenvectors of \( G \) as given in \( (63) \).

Notice that \( \cos(\xi_k) \) is negative for \( k \) odd and positive for \( k \) even. Thus, each term of \( (70) \) includes a dominant positive part and a small negative part. Let us separate them and write
\[ K = K_1 - K_2, \quad (74) \]

where \( K_1 \) includes the dominant part and \( K_2 \) includes the small part of each term. Both \( K_1 \) and \( K_2 \) are self-adjoint and positive. The odd terms of \( K_1 \) are given by

\[
\int_0^1 \frac{\cos (\theta_k) \left( 1 + \cos (\theta_k) \right) \delta_1(\xi_k)}{2\delta_0(\xi_k)} \left[ \cos \left( \frac{\xi_k x}{2a} \right) \cos \left( \frac{\xi_k y}{2a} \right) \right] \, d\mu, \quad (75a)
\]

where

\[
ad_1(\xi_k) = a \left[ 1 + \frac{\sin (\xi_k)}{\xi_k} \right] = \int a \cos \left( \frac{\xi_k y}{2a} \right) \, ds, \quad (75b)
\]

is a normalization factor. The even terms can likewise be written

\[
\int_0^1 \frac{\cos (\theta_k) \left( 1 + \cos (\theta_k) \right) \delta_2(\xi_k)}{2\delta_0(\xi_k)} \left[ \sin \left( \frac{\xi_k x}{2a} \right) \sin \left( \frac{\xi_k y}{2a} \right) \right] \, d\mu, \quad (76a)
\]

where

\[
ad_2(\xi_k) = a \left[ 1 - \frac{\sin (\xi_k)}{\xi_k} \right] = \int a \sin \left( \frac{\xi_k y}{2a} \right) \, ds, \quad (76b)
\]

is another normalizing factor. Equation (72) implies that \( \theta_k \) moves over a very short range as \( \mu \) integrates from 0 to 1. The mean value theorem allows us to write (75a) and (76a) as

\[
\cos \left( \frac{\xi_k x}{2a} \right) \cos \left( \frac{\xi_k y}{2a} \right) \int_0^1 \frac{\cos (\theta_k) \left( 1 + \cos (\theta_k) \right) \delta_1(\xi_k)}{2\delta_0(\xi_k)} \, d\mu, \quad (77a)
\]

for \( k \) odd and

\[
\sin \left( \frac{\xi_k x}{2a} \right) \sin \left( \frac{\xi_k y}{2a} \right) \int_0^1 \frac{\cos (\theta_k) \left( 1 + \cos (\theta_k) \right) \delta_2(\xi_k)}{2\delta_0(\xi_k)} \, d\mu, \quad (77b)
\]

for \( k \) even, where

\[
\xi_k (1, 1) = \xi_k (1, 1) = \left\{ k \pi, \frac{-k \pi}{2a}, k \pi \right\}, \quad (77c)
\]

The terms that have been extracted from the integrals in (77a,b) represent the normalized outer product of the eigenvectors of \( K_1 \). The eigenvalues are approximated by evaluating the integrals. First, notice that from (67) we have

\[
\tan (\theta_k) = \tan (\theta_k) = \theta_k \quad (78)
\]

Solving (78) for \( \theta_k \) yields.
\[
\theta_k = \left( \frac{k \pi}{2a} \right) \left( \frac{1}{1 + \frac{\mu}{2a}} \right).
\] (79)

Next, notice that for \( k \) odd
\[
\frac{\delta_1(\xi_k)}{\delta_0(\xi_k)} = \frac{1 + \frac{\sin(\theta_k)}{\xi_k}}{1 - \frac{\sin(2\xi_k)}{2\xi_k}} = \frac{1 + \frac{\sin(\theta_k)}{k \pi - \theta_k}}{1 + \frac{\sin(2\theta_k)}{2(k \pi - \theta_k)}} = \left( 1 + \frac{1}{2} \frac{\theta_k}{k \pi} \right).
\]

Expanding the remaining terms to second powers of \( \theta_k \) yields
\[
\frac{1}{\cos(\theta_k)(1 + \cos(\theta_k))} \delta_1(\xi_k) \delta_0(\xi_k) d\mu = \frac{1}{0} \left( 1 - \frac{3}{4} \theta_k^2 \right) d\mu = 1 - \frac{1}{4} \left( 1 + \frac{1}{2a} \right) \left( \frac{k \pi}{2a} \right)^2.
\] (80)

The term for \( k \) even yields the same result. We have established an asymptotic form for the eigenvectors \( u_k^{(1)} \) of \( K_1 \), namely
\[
u_k^{(1)} = \begin{cases} \cos \left( \frac{\xi_k}{2a} \right), & \text{\( k \) odd}, \\
\sin \left( \frac{\xi_k}{2a} \right), & \text{\( k \) even} \end{cases}
\] (81)

where \( \xi_k = \frac{k \pi}{2}, \frac{k \pi}{2a}, \frac{k \pi}{2}, \frac{k \pi}{2a}, \) and the eigenvalues \( \sigma_k^{(1)} \) of \( K_1 \), namely
\[
\sigma_k^{(1)} = 1 - \frac{1}{4} \left( \frac{k \pi}{2a} \right)^2.
\] (82)

The odd terms of \( K_1 \) are given by
\[
\frac{1}{0} \cos(\theta_k)(1 - \cos(\theta_k)) \delta_1(\xi_k) d\mu = \delta_{\theta_k}(\xi_k) \frac{\xi_k}{2a} d\mu.
\] (83a)

and the even terms are given by
\[
\frac{1}{0} \cos(\theta_k) \delta_0(\xi_k) \cos(\theta_k) d\mu = \delta_{\theta_k}(\xi_k) \frac{\xi_k}{2a} d\mu.
\] (83b)

Applying the mean value theorem, we write (83a) and (83b) as
for \( k \) odd and

\[
\sin \left( \frac{\pi x_k}{2a} \right) \cos \left( \frac{\pi y_k}{2a} \right)
\]

\[
\frac{1}{d \delta_2(\xi_k)} \int_0^1 \cos (\theta_k)(1 - \cos (\theta_k)) \delta_2(\xi_k) d\mu,
\]

for \( k \) even, where

\[
\xi_k(x, y), \ \eta_k(x, y) \in [k \pi - \frac{k \pi}{2}, k \pi] .
\]

As before, the terms extracted from the integrals represent the normalized outer product of the eigenvectors of \( K_2 \). The eigenvalues are approximated by evaluating the integrals in (84a,b). This yields

\[
\sigma_{k}^{(2)} = \frac{1}{2} \int_0^1 \cos (\theta_k)(1 - \cos (\theta_k)) \delta_1(\xi_k) d\mu = \int_0^1 0_k^2 - \frac{1}{4} 0_k^4 d\mu
\]

\[
= \frac{1}{12} \left( \frac{k \pi}{2} \right) - \frac{1}{12} \left( \frac{k \pi}{2} \right)^2,
\]

(85)

To find approximations to the eigenvalues of \( K \), we must consider both \( K_1 \) and \( K_2 \). One can show that \( \xi_k \) and \( \eta_k \) in (81) are given approximately by setting \( \mu = 1 \pm (1 + \frac{1}{8a}) \) in (67), that is, by the roots of

\[
\frac{1}{2} (1 + \frac{1}{8a}) \xi_k = \tan \left( \xi_k \right)
\]

(86)

Using these values of \( \xi_k \) in (81) yields approximate eigenvectors \( u_k \) of \( K \). The approximate eigenvalues are found from

\[
\sigma_k = \frac{1}{0_k} \frac{K_{0_k} u_k}{u_k}, \quad \frac{K_{0_k} u_k}{u_k}, \quad \frac{K_{0_k} u_k}{u_k}, \quad \frac{K_{0_k} u_k}{u_k},
\]

(87)

The first term on the left of (87) is given by (82). The second term requires some work. Suppose \( k \) is odd. Then, \( u_k \cdot \cos (\frac{\pi x_k}{2a}) \) is orthogonal to all the odd terms in the expansion of \( K_2 \). Consider an even term of \( K_2 \). The eigenvector of \( K_2 \), \( u_k \), \( \cdot \cos (\frac{\pi y_k}{2a}) \). We have from (81b) and (81c)

\[
\int_0^1 \cos \left( \frac{\pi x_k}{2a} \right) \cos \left( \frac{\pi y_k}{2a} \right) d\mu = \int_0^1 \frac{1}{2} \frac{1}{2} d\mu = \frac{1}{4} \frac{1}{4}
\]

(88)

Thus, using (88) we have
\[
\frac{\langle K_{\beta} h_k h_k \rangle}{\langle h_k h_k \rangle} = \sum_{i \text{ even}} \sigma_{i} \left( \frac{2}{\pi} \right)^2 \frac{(2k)^2}{(k^2 - l^2)^2} = \frac{1}{3a^2} \sum_{i \text{ even}} \frac{k^2 l^2}{(k^2 - l^2)^2}.
\] (89)

The sum in (89) can be bounded above and below by

\[
\sum_{i \text{ even}} \frac{k^2 l^2}{(k^2 - l^2)^2} \leq \frac{k-1}{2} \int_{0}^{1} \frac{w^2}{(1 - w^2)^2} dw = \frac{k}{2} \int_{0}^{1} \frac{w^2}{(1 - w^2)^2} dw
\] (90a)

\[
\sum_{i \text{ even}} \frac{k^2 l^2}{(k^2 - l^2)^2} \geq \frac{k}{2} \int_{0}^{1} \frac{w^2}{(1 - w^2)^2} dw + \left[ \frac{k^2 (k - 1)^2}{(k^2 - (k - 1)^2)^2} + \frac{k^2 (k + 1)^2}{(k^2 - (k + 1)^2)^2} \right] + \frac{k}{2} \int_{k}^{1} \frac{w^2}{(1 - w^2)^2} dw.
\] (90b)

The integrals in (90) become

\[
\frac{k-1}{2} \int_{0}^{1} \frac{w^2}{(1 - w^2)^2} dw = \frac{k^2}{4} \left[ \frac{k - 1}{2k - 1} - \frac{\ln |2k - 1|}{2k} \right]
\] (91a)

and

\[
\frac{k}{2} \int_{k}^{1} \frac{w^2}{(1 - w^2)^2} dw = \frac{k^2}{4} \left[ \frac{k + 1}{2k + 1} + \frac{\ln |2k + 1|}{2k} \right].
\] (91b)

Putting (91a,b) into (90a,b) and rearranging into (89) yields

\[
\frac{\langle K_{\beta} h_k h_k \rangle}{\langle h_k h_k \rangle} = \frac{1}{3a^2} \left[ \frac{k \pi}{2a} \right]^2 \left[ \frac{k \pi}{2a} \right]^{2} \left[ \frac{1}{2} \right] + \frac{1}{2} \left[ \frac{1}{2} \right] + \frac{1}{2} \left[ \frac{1}{2} \right]
\] (92a)

\[
\langle K_{\beta} h_k h_k \rangle \cdot \langle h_k h_k \rangle = \frac{1}{3a^2} \left[ \frac{k \pi}{2a} \right]^2 \left[ \frac{1}{2} \right] + \frac{1}{2} \left[ \frac{1}{2} \right] + \frac{1}{2} \left[ \frac{1}{2} \right]
\] (92b)

Since the term in brackets in (92a) is very nearly unity, we make the approximation
\[
\frac{1}{3\pi^2} \left[ \frac{k\pi}{2a} \right]^2 \leq \frac{\langle K - \mu \rangle}{\langle \mu \rangle} \leq \frac{1}{\pi^2} \left[ \frac{k\pi}{2a} \right]^2
\]  

(93)

Combining (93) with (82) into (87) yields the approximate eigenvalue \(\sigma_k\) of \(K\), namely

\[
1 - \left[ \frac{1}{4} - \frac{1}{\pi^2} \right] \left[ \frac{k\pi}{2a} \right]^2 \leq \sigma_k \leq 1 - \left[ \frac{1}{4} - \frac{1}{3\pi^2} \right] \left[ \frac{k\pi}{2a} \right]^2
\]  

(94)

Now suppose \(k\) is odd in (87). We have \(u_k = \sin \left( \frac{\xi_k x}{2a} \right)\), which is orthogonal to all of the odd terms of \(K_2(u_l) = \cos \left( \frac{\xi_l x}{2a} \right)\) for \(l\) odd. The even terms of \(K_2\) yield an expansion identical to (88) above. Thus, (94) holds for \(k\) odd as well.

Notice that \(\frac{1}{4} + \frac{1}{3\pi^2} \approx .2838\) and \(\frac{1}{4} + \frac{1}{\pi^2} \approx .3513\). Compare this with the eigenvalues of \(G\) as given in (64) and (65) and the compare eigenvectors as given in (62) and (63) with the eigenvector approximations (81). Notice that the eigenvalues of \(G\) have asymptotic form

\[
\lambda_k \approx 1 - \frac{1}{3} \left[ \frac{k\pi}{2a} \right]^2
\]  

(95)

Now, for \(\frac{k\pi}{2a} \gg 1\), the roles of \(\sin\) and \(\cos\) in (70) are reversed. For \(k\) odd \(\sin \left( \frac{\xi_k x}{2a} \right)\) dominates and for \(k\) even \(\cos \left( \frac{\xi_k x}{2a} \right)\) dominates where \(\xi_k, \xi_k\) are near \((k - \frac{1}{2})\pi\). This is so in spite of the fact that the integration with respect to \(\mu\) sweeps through almost all values in the interval \([(k - \frac{1}{2})\pi, k\pi]\). The major portion of the integral involves the left end of the interval. Here, the terms decay like \(\ln \left( \frac{k\pi}{2a} \right)\). The eigenvalues decay at a faster rate.

Suppose we denote the eigenvector decomposition of \(K\) and \(G\) by

\[
K = U \Sigma U^*, \quad \Sigma = \text{diag} (\sigma_i)_i
\]  

(96a)

\[
G = V \Lambda V^*, \quad \Lambda = \text{diag} (\lambda_i)_i
\]  

(96b)

where \(U\) and \(V\) are unitary operators. As the discussion above indicates, and numerical experiments support, \(U^*\) and \(V\) are very similar, especially for the large eigenvalues. We have

\[
V^*U = I + \Lambda
\]  

(97)

where \(\Lambda\) is small. Now consider

\[
(1 - G)^{-1} K (1 - G)^{-1} (1 - G)^{-1} K (1 - G)^{-1} (1 - G)^{-1} (G^*)^k (G^*)^k
\]  

(98)

from Eq. (11). Using (96a,b) we have
\[(I - G)^{-1}(K - G) = V(I - \Lambda)^{-1}V^* (U^*U^* - V\Lambda V^*) = V(I - \Lambda)^{-1}(U^*U^*)V^* - (U^*V^*)\Lambda V^*\]

Substitution of (97) yields

\[(1 - G)^{-1}(K - G) = V(I - \Lambda)^{-1}(\Sigma - \Lambda) V^* + V(I - \Lambda)^{-1}(\Delta(\Sigma - \Lambda) + (I + \Delta)(\Sigma - \Delta\Lambda)) V^*\]  

(99)

Notice that the second term is small because for large eigenvalues, \(\Sigma - \Lambda\) and \(\Delta\) are small. For small eigenvalues, \(\Sigma\) and \(\Delta\) are both small. Thus, the first term is a good approximation. We have

\[(I - \Lambda)^{-1}(\Sigma - \Lambda) = \text{diag} (\cdots \rho_k \cdots) ,\]  

(100)

where

\[\rho_k = \frac{\sigma_k - \lambda_k}{1 - \lambda_k} .\]  

(101)

Using the asymptotic form of both \(\sigma_k\) (94) and \(\lambda_k\) (95) yields

\[-0.0539 = \left[\frac{1}{4} - \frac{3}{\pi^2}\right] \leq \rho_k \leq \left[\frac{1}{4} - \frac{1}{\pi^2}\right] = 0.1487 .\]  

(102)

Of course, this is never achieved in practice due to the differences in the eigenvectors of \(G\) and \(K\) (which are reflected in \(\Lambda\)), the pollution due to intermediate eigenvalues, and perhaps most importantly, perturbations due to discretization.

The exact form of \(\lambda_k\) is given in (64). The intermediate eigenvalues of \(K\) can be approximated by

\[|\cos (\zeta_k)| \left[\frac{1 + |\cos (\zeta_k)|}{2}\right] , \quad \zeta_k = \tan (\zeta_k) .\]  

(103)

as the equations (77a,b) suggest. A plot of numerically computed values \(\sigma_k, \lambda_k, \text{ and } \rho_k\) against \(\frac{k}{a}\) appears in Fig. 3. Here \(a = 32\) was used. The curves for various values of \(a\) are similar, as are the values using analytic \(\lambda_k\) and approximate \(\sigma_k\). Notice that the maximum value of \(\rho_k\) is approximately 0.23. This corresponds to the findings in [1.4.1].

13 OTHER PRECONDITIONINGS

Also notice that in Fig. 1 the eigenvalues of \(K\) decrease as \(\frac{1}{k}\), while those of \(G\) decrease as \(\frac{1}{k^2}\). One would expect to do much better if one used as a preconditioner an operator whose spectrum more closely fits the spectrum of \(K\). For example, one might consider using a preconditioning based upon the eigenvectors of \(G\), which are given in (63), and the eigen
value approximations in (103). This leads to a preconditioning, $G$, for which the spectral radius of

$$
\hat{S} = (I - \hat{G})^{-1}(K - \hat{G})
$$

is on the order of .06. However, computation with such an operator is very expensive. Another preconditioning with attractive properties for problems with very large $a$ is based upon the fast Fourier transform (FFT). Suppose, for example, that $k = 100$ frequencies are sufficient to resolve the solution. Further, suppose that $(100 \frac{\pi}{2a}) \ll 1$. The analysis of Sec. 12 indicates that the eigenvectors of $K$ are given by (81), that is, are very nearly Fourier vectors on a somewhat larger region. To find that region consider the very first eigenvector of the diffusion operator. We have from (60a,b)

$$
\frac{\beta}{a} \eta_1 = \cot (\eta_1) .
$$

Suppose we let $\eta_1 = \frac{\pi}{2} - 0_1$. Then (105) becomes

$$
\frac{\beta}{a} \left[ \frac{\pi}{2} - 0_1 \right] = 0_1 ,
$$

which yields

$$
0_1 - \frac{\pi \beta}{2a} , \eta_1 : \frac{\pi}{1 + \frac{\beta}{a}} .
$$

Now the end point of the larger region occurs where $\eta_1 = \frac{\pi}{a}$, which yields
Recall that \( \beta = 0.7 \) gave the best results for \( a = 1 \) (see Fig. 2). This is very close to the extrapolated end point for the semi-infinite slab [Wi]. For \( a \) large, the significance of this extended region diminishes. We shall give numerical results using this preconditioning in a future report.

14 NUMERICAL RESULTS

The operators \( K \) and \( G_\beta \) were constructed using a finite element discretization on a mesh using 200 points. Eigenvector/value decompositions were performed to support the analysis of Sec. 11 and Sec. 12. Of course, only the first half of the eigenvectors and eigenvalues have any chance at accuracy. Over a large range of values of the boundary parameter \( \beta \) and the slab width \( a \), the initial eigenvectors and eigenvalues behaved as predicted. The eigenvalues of \( K \) satisfy a relationship of the form

\[
1 - \delta(a,k) \left( \frac{k\pi}{2a} \right)^2
\]

for \( \left( \frac{k\pi}{2a} \right) \ll 1 \), where \( \delta(a,k) \) varies slowly with \( k \) and \( a \). Table 1 contains values of \( \delta \) for various values of \( k \) and \( a \). The numbers in bold print correspond to values of \( k \) and \( a \) with \( \frac{k\pi}{2a} \approx 1 \). The values for \( 8 \leq a \leq 128 \) were calculated on using 200 mesh points. The values for \( a = 256 \) were calculated using 500 mesh points. The values of \( \delta(a,k) \) fit the bounds given in (94) fairly well for \( \frac{k\pi}{2a} \leq \frac{1}{2} \).

Also, the DSA preconditioning alone, that is using \((I - G)\) as a preconditioning for \((I - K)\) in the Neumann series, was compared with using DSA in a preconditioned conjugate gradient iteration (PCG). This produced surprising results. The conjugate gradient iteration performed better than predicted from bounds like (56). The bound (56) is only a bound and presumes even distribution of eigenvalues throughout the interval that contains the spectrum of \((I - G)^{-1}(I - K)\). The conjugate gradient algorithm has the capacity to take advantage of the distribution of the eigenvalues (cf. [HeSt]). For example, Table 2 contains a comparison of the relative residual for DSA alone, the expected relative residual using DSA with the PCG iteration and the actual relative residual using DSA with PCG. Here \( a = 128, \beta = \frac{2}{3} \), and a mesh of 200 points was used.

15 SUMMARY

We have shown that standard notions of linear algebra can provide a framework for the discussion of algorithms for the numerical solution of the transport equation. In particular, we have seen that the DSA algorithm is the Neumann series applied to the standard integral
Table 1. VALUES OF δ VERSUS k

<table>
<thead>
<tr>
<th></th>
<th>8</th>
<th>16</th>
<th>32</th>
<th>64</th>
<th>128</th>
<th>256</th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.2764</td>
<td>0.3047</td>
<td>0.3216</td>
<td>0.3365</td>
<td>0.3558</td>
<td>0.3672</td>
</tr>
<tr>
<td>2</td>
<td>0.2628</td>
<td>0.3002</td>
<td>0.3203</td>
<td>0.3366</td>
<td>0.3575</td>
<td>0.3568</td>
</tr>
<tr>
<td>3</td>
<td>0.2432</td>
<td>0.2931</td>
<td>0.3182</td>
<td>0.3358</td>
<td>0.3576</td>
<td>0.3548</td>
</tr>
<tr>
<td>4</td>
<td>0.2206</td>
<td>0.2837</td>
<td>0.3153</td>
<td>0.3350</td>
<td>0.3575</td>
<td>0.3541</td>
</tr>
<tr>
<td>5</td>
<td>0.1976</td>
<td>0.2725</td>
<td>0.3116</td>
<td>0.3540</td>
<td>0.3572</td>
<td>0.3537</td>
</tr>
<tr>
<td>10</td>
<td>0.1095</td>
<td>0.2077</td>
<td>0.2846</td>
<td>0.3256</td>
<td>0.3548</td>
<td>0.3526</td>
</tr>
<tr>
<td>20</td>
<td>—</td>
<td>0.1122</td>
<td>0.2145</td>
<td>0.2966</td>
<td>0.3452</td>
<td>0.3500</td>
</tr>
<tr>
<td>40</td>
<td>—</td>
<td>—</td>
<td>0.1449</td>
<td>0.2223</td>
<td>0.3131</td>
<td>0.3453</td>
</tr>
<tr>
<td>80</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>0.1173</td>
<td>0.2996</td>
<td>0.3258</td>
</tr>
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</table>

Table 2. RELATIVE RESIDUAL VERSUS ITERATION COUNT

<table>
<thead>
<tr>
<th>Iteration</th>
<th>DSA Alone</th>
<th>Expected PCG</th>
<th>Actual PCG</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.23</td>
<td>0.65</td>
<td>-1</td>
</tr>
<tr>
<td>2</td>
<td>0.53</td>
<td>0.43</td>
<td>-1</td>
</tr>
<tr>
<td>3</td>
<td>0.12</td>
<td>0.28</td>
<td>-3</td>
</tr>
<tr>
<td>4</td>
<td>0.28</td>
<td>0.18</td>
<td>-2</td>
</tr>
<tr>
<td>5</td>
<td>0.64</td>
<td>0.12</td>
<td>-3</td>
</tr>
<tr>
<td>6</td>
<td>0.14</td>
<td>0.76</td>
<td>-3</td>
</tr>
<tr>
<td>7</td>
<td>0.34</td>
<td>0.18</td>
<td>-3</td>
</tr>
<tr>
<td>8</td>
<td>0.78</td>
<td>0.76</td>
<td>-5</td>
</tr>
<tr>
<td>9</td>
<td>0.18</td>
<td>0.23</td>
<td>-5</td>
</tr>
<tr>
<td>10</td>
<td>0.41</td>
<td>0.23</td>
<td>-6</td>
</tr>
</tbody>
</table>

equation formulation, Eq. (7), preconditioned by a certain diffusion operator \((T - \gamma l)\) given in Sec. 8. We have also seen that the boundary conditions can be handled straightforwardly.

The boundary conditions (cf. (23))

\[
B \phi_{n+1} = RK \gamma \psi_n = BLH^{-1} \gamma \phi_n = BL \psi_n
\]

can be thought of as expressing the fact that the prescribed boundary values of \(\phi\) after the accelerated part of the scheme, \(\phi_{n+1}\), should remain the same as the values of \(\phi\) before the acceleration, \(L \psi_n\). Again this agrees completely with the boundary conditions used in [Lal].

Using the spectral properties of the integral formulation of \(K\) and the DSA operator \(G\), we have demonstrated why DSA works well for optically dense problems (i.e., large \(\alpha\)). We have used this approach to suggest other preconditionings, \((I - G)\), and iteration schemes whose convergence rates depend upon the spectrum of a fixed operator \((I - G) (I - K)\).
Finally, we have demonstrated analytically in Sec. 9 that iterative acceleration of the basic Neumann iteration (13) can produce profound speedup. Also, we have demonstrated numerically that the PCG algorithm can produce significant acceleration of the DSA preconditioning.

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REFERENCES


