INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING, VOL. 41, 875–898 (1998)

PRECONDITIONED KRYLOV SUBSPACE METHODS FOR BOUNDARY ELEMENT SOLUTION OF THE HELMHOLTZ EQUATION

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ABSTRACT

Discretization of boundary integral equations leads, in general, to fully populated complex valued non-Hermitian systems of equations. In this paper we consider the efficient solution of these boundary element systems by preconditioned iterative methods of Krylov subspace type. We devise preconditioners based on the splitting of the boundary integral operators into smooth and non-smooth parts and show these to be extremely efficient. The methods are applied to the boundary element solution of the Burton and Miller formulation of the exterior Helmholtz problem which includes the derivative of the double layer Helmholtz potential—a *hypersingular* operator. © 1998 John Wiley & Sons, Ltd.

Int. J. Numer. Meth. Engng., **41**, 875–898 (1998)

KEY WORDS: preconditioned Krylov subspace methods; conjugate gradient; boundary integral equations; hypersingular operator; Helmholtz equation

1. INTRODUCTION

Many boundary value problems of mathematical physics and engineering are now commonly reformulated as integral equations over the boundary of the domain of interest and subsequently solved by finite element type methods; see References 1–3 (and references therein). On smooth domains general linear boundary integral equations of interest fall into the category of Fredholm first kind, Fredholm second kind, hypersingular (integro-differential) and Cauchy singular equations. Each of these equations have very distinctive characteristics and their analytical and numerical studies have traditionally received completely different treatments. However, they may be viewed as *pseudodifferential* operator equations over appropriate Sobolev spaces and written as $\mathscr{A}\phi = f$, where $\mathscr{A} : \mathscr{H}^r(\Gamma) \to \mathscr{H}^{r-\alpha}(\Gamma)$ is a strongly elliptic, injective operator of order α and Γ is the boundary of the domain of interest, see Reference 4. The *pseudodifferential* concept allows the study of differential and integral operators within the same algebras of operators.[5, 6] In this framework much of the properties of the boundary integral operators and convergence analyses of ensuing numerical methods can be studied in a unified fashion, see Reference 7.

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CCC 0029–5981/98/050875–24$17.50

Received 4 October 1996
Revised 4 April 1997

Discretization of boundary integral equations using spline approximation spaces leads to dense linear systems $\mathscr{A}_n\phi_n = f_n$, where n denotes the number of degrees of freedom. For consistency with the linear algebra content of this paper at times we represent these linear systems in the generic form $A\mathbf{x} = \mathbf{b}$, $A \in \mathbb{C}^{n\times n}$. For large n the cost of their solution by direct methods becomes prohibitive. Much research has been carried out into the development of efficient iterative solutions for boundary element systems; see for example References 8–11 and references therein. In this paper we are primarily concerned with the efficient solution of these boundary element equations by preconditioned Krylov subspace methods. We must point out that recently a number of more specialized schemes such as wavelet-based approximations[12, 13] or the multipole algorithm[14] and the sparse approximation methods[15] have been proposed which essentially approximate the boundary element system with one with $\mathcal{O}(n)$ non-zero elements, leading to efficient methods with linear computational complexity. We will not discuss such schemes here.

Although originally developed for the fast solution of large and sparsely populated systems arising from finite difference and finite element discretizations, iterative methods such as multi-grid and conjugate gradient type schemes have been used for boundary element equations; see Reference 16 (and references therein). For the case of second kind Fredholm equations where $\mathscr{A} = \lambda\mathscr{I} - \mathscr{K}$ and $\mathscr{K}$ is a compact integral operator, corresponding to $\alpha = 0$, these schemes have been shown to be efficient; see for example References 17–19. This is essentially because the eigenvalues of $\mathscr{A}_n$ cluster in the vicinity of λ, due to the compactness of $\mathscr{K}$. This clustering of the eigenvalues is the ideal situation for many iterative methods.

For the case of first kind Fredholm equations where $\mathscr{A} = \mathscr{K}$ is compact with a weakly singular or logarithmic kernel, corresponding to $\alpha = -1$, the eigenvalues cluster around zero, leading to an ill-conditioned linear system. On the other hand, for the hypersingular case, corresponding to $\alpha = +1$, there is no true clustering of the eigenvalues, as they grow with n; see Section 3 and Appendix I. Also for the case of Cauchy singular equations, corresponding to $\alpha = 0$, the eigenvalues remain bounded with no point of accumulation. In these cases modifications to the linear equations are necessary in order to avoid divergence or to speed up the convergence of iterative methods such as multi-grid or conjugate gradient type.[20, 21]

In this paper we study the convergence of three iterative methods of the conjugate gradient type, belonging to the Krylov subspace class, as applied to boundary element equations. Methods in this class perform well whenever there is clustering of the eigenvalues or singular values of A away from zero. We devise preconditioners D, based on the splitting of A as $D - C$, which results in the clustering of the eigenvalues of $D^{-1}A$. The matrix D represents the discretization of the most dominant part of $\mathscr{A}$, with the restriction that the solutions of systems $D\mathbf{w} = \mathbf{t}$ can be performed cheaply. Essentially, we solve with Krylov subspace methods the system $B\mathbf{x} = D^{-1}\mathbf{b}$, where $B = I - D^{-1}C$ with its eigenvalues clustered at unity.

Here we concentrate on the boundary integral solution of the exterior Helmholtz equation where the source of difficulty is the presence of the hypersingular operator, the normal derivative of the double layer Helmholtz potential. In Section 2 we introduce boundary integral equations for the Helmholtz problem. In Section 3 we study the mapping properties and spectral behaviour of the Helmholtz integral operators. In Section 4 our iterative schemes and preconditioners are introduced and analysed, and we present the results of numerical experiments in Section 5. Furthermore, in Appendix I we derive analytically the eigenvalues of the derivative of the double layer Laplacian potential, and those of its matrix approximation. These results are used in Section 5. For completeness, we present in Appendix II an outline of the three Krylov subspace algorithms (viz. CGNR, GMRES, Bi-CGSTAB) which we have used in this paper.

2. EXTERIOR HELMHOLTZ PROBLEM

We study the boundary integral solution of the Helmholtz equation

$$(\nabla^2 + k^2)\phi(p) = 0, \quad p \in D_+ \tag{1}$$

in an unbounded domain, D_+, exterior to a smooth $\mathscr{C}^\infty$ boundary Γ, satisfying a general boundary condition on Γ of the form

$$a\frac{\partial \phi}{\partial n}(p) + b\phi(p) = g(p), \quad p \in \Gamma \tag{2}$$

$\partial/\partial n$ denotes differentiation in the direction of the normal to Γ pointing towards D_+. For uniqueness of the solution of (1)–(2) we also require ϕ to satisfy a Sommerfeld type radiation condition (boundary condition at infinity)[22]

$$\frac{\partial \phi}{\partial r} - ik\phi = o(r^{-1/2}), \quad r = |p| \to \infty \tag{3}$$

For scattering problems the total acoustic pressure is the sum of the incident and the scattered field $\phi = \phi^{\text{inc}} + \phi^{\text{sc}}$, and only the scattered field satisfies the radiation condition (3). Without loss of generality we will concentrate on the pure radiation problem ($\phi^{\text{inc}} \equiv 0$).

A careful application of Green's second identity over the unbounded domain D_+, yields the *Helmholtz integral representation formula*

$$\phi(p) = \int_\Gamma \phi(q)\frac{\partial G_k}{\partial n_q}(p,q)\,\mathrm{d}\Gamma_q - \int_\Gamma G_k(p,q)\frac{\partial \phi}{\partial n_q}(q)\,\mathrm{d}\Gamma_q, \quad p \in D_+ \tag{4}$$

for the solution of (1)–(3). In the above $G_k(p,q) = (i/4)H_0^{(1)}(k|p-q|)$ is the free space Green's function for the Helmholtz equation (1) and $H_0^{(1)}$ is the first kind Hankel function of order zero.

The integral representation formula (4) requires the Cauchy data $(\phi, \partial\phi/\partial n)$ on the boundary. The boundary condition (2) gives either ϕ or $\partial\phi/\partial n$ or a relationship between the two in the case of a 'spring-like' scatterer and therefore we need another relationship between the boundary values of ϕ and $\partial\phi/\partial n$ in order to find the Cauchy data.

In direct boundary integral equations, this second relationship is usually obtained by taking the limit as $p \in D_+ \to p \in \Gamma$, in (4). Using the trace properties (jump relations) of the single and double layer potentials, this yields the so-called *surface Helmholtz equation* (SHE)

$$-\frac{1}{2}\phi(p) + \int_\Gamma \phi(q)\frac{\partial G_k}{\partial n_q}(p,q)\,\mathrm{d}\Gamma_q = \int_\Gamma G_k(p,q)\frac{\partial \phi}{\partial n_q}(q)\,\mathrm{d}\Gamma_q, \quad p \in \Gamma \tag{5}$$

which should be used in conjunction with (2) to yield $(\phi, \partial\phi/\partial n)$.

Equation (5) may be written in operator form as

$$\left(-\frac{1}{2}\mathscr{I} + \mathscr{M}_k\right)\phi(p) = \left(\mathscr{L}_k\frac{\partial \phi}{\partial n}\right)(p), \quad p \in \Gamma \tag{6}$$

with obvious definitions for the *single* and *double* layer Helmholtz potentials $\mathscr{L}_k$ and $\mathscr{M}_k$ respectively. In the case of the Neumann boundary condition, replacing the value of $\partial\phi/\partial n$ from (2) into (6) yields a second kind Fredholm integral equation for ϕ, the missing part of the Cauchy data.

On the other hand if Dirichlet data is provided (6) would yield a first kind Fredholm equation for $\partial\phi/\partial n$. In general however, (2) and (6) may need to be solved implicitly to yield ϕ and $\partial\phi/\partial n$.

It is well-known (see References 3 and 23 and references therein) that for any given Γ, there is a countable set $I_{\mathbf{D},\Gamma}$, of real values of the wavenumber k, for which both the operators $-\frac{1}{2}\mathscr{I} + \mathscr{M}_k$ and $\mathscr{L}_k$ are singular. The subscript $\mathbf{D}$ in $I_{\mathbf{D},\Gamma}$ indicates that these so-called *forbidden wave numbers*, are precisely the eigenvalues of the interior **D**irichlet problem.[22, 23] This makes the use of equation (6) unsuitable, at least from a numerical computation point of view, since the boundary integral equation (6) and also its resulting discrete equations become ill-conditioned whenever k is close to $I_{\mathbf{D},\Gamma}$.[24] We shall see shortly that if Γ is a unit circle, then $I_{\mathbf{D},\Gamma} = \{k \,|\, J_n(k) = 0 \text{ for some } n = 0, 1, 2, \ldots\}$, where J_n's are the Bessel functions of integer order n.

A different relationship between the Cauchy data can be obtained by formally differentiating the *surface Helmholtz equation* (6) in the direction of $\mathbf{n}_p$, the normal to Γ at p. This step of differentiating boundary functions in the direction of normal can be justified rigorously.[4, 25] This results in the boundary integral equation

$$(\mathscr{N}_k\phi)(p) = (\tfrac{1}{2}\mathscr{I} + \mathscr{M}_k^{\mathrm{T}})\frac{\partial\phi}{\partial n_p}(p), \quad p \in \Gamma \tag{7}$$

referred to as the *differentiated surface Helmholtz equation*. The operators $\mathscr{M}_k^{\mathrm{T}}$ and $\mathscr{N}_k$ are the normal derivatives of $\mathscr{L}_k$ and $\mathscr{M}_k$ respectively and are defined as

$$(\mathscr{M}_k^{\mathrm{T}}\sigma)(p) = \frac{\partial}{\partial n_p}(\mathscr{L}_k\sigma)(p) = \int_\Gamma \sigma(q)\frac{\partial G_k}{\partial n_p}(p,q)\,\mathrm{d}\Gamma_q$$

and similarly

$$(\mathscr{N}_k\sigma)(p) = \frac{\partial}{\partial n_p}\int_\Gamma \sigma(q)\frac{\partial G_k}{\partial n_q}(p,q)\,\mathrm{d}\Gamma_q = \frac{\partial}{\partial n_p}(\mathscr{M}_k\sigma)(p) \tag{8}$$

Similar to equation (6), for a given boundary Γ, both the operators $\mathscr{N}_k$ and $\frac{1}{2}\mathscr{I} + \mathscr{M}_k^{\mathrm{T}}$ in (7) are also singular for a countable set $I_{\mathbf{N},\Gamma}$, of real values of k. These values are precisely the eigenvalues of the interior **N**eumann problem.[22, 23] For the case of a unit circle $I_{\mathbf{N},\Gamma} = \{k \,|\, J_n'(k) = 0 \text{ for some } n = 0, 1, 2, \ldots\}$.

It was shown by Burton and Miller in Reference 23 that a linear combination of (6) and (7) in the form

$$\left\{-\frac{1}{2}\mathscr{I} + \mathscr{M}_k + i\eta\mathscr{N}_k\right\}\phi(p) = \left\{\mathscr{L}_k + i\eta\left(\frac{1}{2}\mathscr{I} + \mathscr{M}_k^{\mathrm{T}}\right)\right\}\frac{\partial\phi}{\partial n}(p), \quad p \in \Gamma \tag{9}$$

has a unique solution for all real values of k, as an equation for ϕ or $\partial\phi/\partial n$, provided the real coupling parameter $\eta \neq 0$. Indeed η can be a function of p provided $\eta(p)$ remains one-signed for all $p \in \Gamma$. We will represent equation (9) by

$$\mathscr{A}_{k,\eta}\phi = \mathscr{B}_{k,\eta}\partial\phi/\partial n \tag{10}$$

with obvious definitions for the linear operators $\mathscr{A}_{k,\eta}$ and $\mathscr{B}_{k,\eta}$.

It is with the efficient solution of the discrete approximations to (10) that we are concerned here. The presence of the operator $\mathscr{N}_k$ hinders the convergence of iterative methods introduced in

Section 4. It can be shown that

$$\frac{\partial^2 G_k}{\partial n_p \partial n_q}(p,q) = \mathcal{O}(r^{-2}), \quad r = |p-q|, \;\; p,q \in \Gamma$$

If the integro-differential operator $\mathcal{N}_k$ is to be viewed as an integral operator with hypersingular kernel, the integral should be understood and evaluated in the sense of the Hadamard *finite part*, see for example References 26–28.

3. SPECTRAL PROPERTIES OF THE HELMHOLTZ OPERATORS

The mapping properties of the Helmholtz integral operators will be studied with emphasis on the spectral properties of these operators for the case where Γ is a unit circle. This allows us a deeper insight into the behaviour of these continuous operators and their discrete counterparts. This is crucial in the analysis of the iterative methods for the boundary element equations.

Following Reference 29, if we assume a global 2π periodic mapping from Γ to $[0, 2\pi]$, the space of $\mathscr{H}^r(\Gamma)$ is equivalent to the space $\mathscr{H}^r[0, 2\pi]$ of 2π periodic distributions, which can then be elegantly defined in terms of Fourier coefficients. Let the 2π periodic complex valued scalar function $\phi \in \mathscr{L}^2[0, 2\pi]$ have the Fourier expansion

$$\phi(t) = \frac{1}{\sqrt{2\pi}} \sum_{m \in \mathbb{Z}} \widehat{\phi}_m \mathrm{e}^{imt}$$

where the Fourier coefficients are given by

$$\widehat{\phi}_m = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \phi(t) \mathrm{e}^{-imt} \, \mathrm{d}t$$

Then, $\mathscr{H}^r[0, 2\pi]$ for any $r \in [0, \infty)$ is the subspace of all 2π periodic distributions in $\mathscr{L}^2[0, 2\pi]$ such that

$$\|\phi\|^2_{\mathscr{H}^r} = \sum_{m \in \mathbb{Z}} (1 + m^2)^r |\widehat{\phi}_m|^2 < \infty$$

$\mathscr{H}^0 \equiv \mathscr{L}^2$ and the spaces $\mathscr{H}^r$ for $r < 0$ are defined by duality with $\mathscr{H}^{-r}$. The following theorem states the essential properties of the four operators that we need in our analysis here.[4, 30, 31]

Theorem 1. The Helmholtz boundary integral operators $\mathscr{L}_k$ and $\mathscr{M}_k$ and their normal derivatives are all strongly elliptic pseudodifferential operators with integer orders. $\mathscr{L}_k, \mathscr{M}_k, \mathscr{M}_k^{\mathrm{T}} : \mathscr{H}^r \to \mathscr{H}^{r-\alpha}$ with order $\alpha = -1$, and $\mathscr{N}_k : \mathscr{H}^r \to \mathscr{H}^{r-\alpha}$ with $\alpha = +1$ are continuous mappings for all $r \in \mathbb{R}$. Furthermore, $\mathscr{A}_{k,\eta} : \mathscr{H}^r \to \mathscr{H}^{r-1}$ and $\mathscr{B}_{k,\eta} : \mathscr{H}^r \to \mathscr{H}^r$ are strongly elliptic continuous bijective mappings.

To gain valuable insight into the spectral properties of these operators we consider the case where the boundary Γ is a unit circle. We state the complete set of eigenfunction–eigenvalues for these operators in the following theorem, the proof of which may be found in References 32 and 31; see also References 33 for similar results in 3-D with Γ a unit sphere.

Theorem 2. For $n = 0, 1, 2, \ldots$

$$\mathscr{L}_k e^{\pm in\theta} = \left\{ \frac{i\pi}{2} J_n(k) H_n(k) \right\} e^{\pm in\theta} = \lambda_{\mathscr{L}_k, n} e^{\pm in\theta}$$

$$\begin{aligned} \mathscr{M}_k e^{\pm in\theta} &= \left\{ -\frac{1}{2} + \frac{i\pi}{2} k J_n'(k) H_n(k) \right\} e^{\pm in\theta} \\ &= \left\{ \frac{1}{2} + \frac{i\pi}{2} k J_n(k) H_n'(k) \right\} e^{\pm in\theta} \\ &= \lambda_{\mathscr{M}_k, n} e^{\pm in\theta} = \lambda_{\mathscr{M}_k^{\mathrm{T}}, n} e^{\pm in\theta} \end{aligned}$$

$$\mathscr{N}_k e^{\pm in\theta} = \left\{ \frac{i\pi}{2} k^2 J_n'(k) H_n'(k) \right\} e^{\pm in\theta} = \lambda_{\mathscr{N}_k, n} e^{\pm in\theta}$$

$\lambda_{\mathscr{A}, n}$ denotes the nth eigenvalue of the operator $\mathscr{A}$. $H_n = H_n^{(1)} = J_n + iY_n$ is the Hankel function of the first kind of order n with J_n and Y_n the Bessel functions of the first and second kind (Neumann function) respectively.

Remark 3. The sets $I_{\mathbf{N},\Gamma}$ and $I_{\mathbf{D},\Gamma}$ given in Section 2 follow directly from Theorem 2.

Also from Theorem 2 it follows that the eigenvalues of $\mathscr{A}_{k,\eta}$ and $\mathscr{B}_{k,\eta}$ in equation (10) are given by

$$\lambda_{\mathscr{A}_{k,\eta}, n} := \lambda_n = \frac{i\pi}{2} k H_n'(k) \{ J_n(k) + i\eta k J_n'(k) \} \tag{11}$$

and

$$\lambda_{\mathscr{B}_{k,\eta}, n} := \mu_n = \frac{i\pi}{2} H_n(k) \{ J_n(k) + i\eta k J_n'(k) \} \tag{12}$$

Using appropriate asymptotic expansions it is shown in Reference 31 that as $n \to \infty$

$$\lambda_{\mathscr{L}_k, n} = \frac{1}{2n} + \mathscr{O}\left(\frac{k^2}{n^3} \right)$$

$$\lambda_{\mathscr{M}_k, n} = \frac{k^2}{4n^3} + \mathscr{O}\left(\frac{k^2}{n^5} \right)$$

$$\lambda_{\mathscr{N}_k, n} = -\frac{n}{2} + \mathscr{O}\left(\frac{k^2}{n} \right)$$

The fact that the eigenvalues of $\mathscr{L}_k$ go to zero as $\mathscr{O}(n^{-1})$ and those of $\mathscr{N}_k$ go to infinity as $\mathscr{O}(n)$ indicate precisely that these are pseudodifferential operators of orders -1 and $+1$ respectively, in agreement with Theorem 1. The result $\lambda_{\mathscr{M}_k, n} = \mathscr{O}(n^{-3})$ indicates that when the boundary is a circle the $\mathscr{M}_k$ operator is smoother than expected and has order -3.

From the above results it follows that

$$\lambda_n \approx -\frac{1}{2} - i\eta \frac{n}{2}$$

and

$$\mu_n \approx \frac{1}{2n} + \frac{i\eta}{2}$$

for large n. Note that $\lambda_n \approx -n\mu_n$.

Using (11)–(12) it can be shown that choosing the coupling parameter η as equal to $1/k$, 'almost minimizes' the condition numbers of the operators $\mathscr{A}_{k,\eta}$ and $\mathscr{B}_{k,\eta}$ simultaneously.[31–33] It was shown in Reference 31 that $\eta = 1/k$ ensures that the early eigenvalues of these operators are moved away from zero, hence improving the conditioning of these normal operators. To be precise it is shown that with $\eta = 1/k$, for small values of n, $\lambda_n = -1 + \mathcal{O}(k^{-1})$ and $\mu_n = i/k + \mathcal{O}(k^{-2})$. We shall see later that this choice of the coupling parameter plays an important role in the speed of convergence of the iterative methods.

4. KRYLOV SUBSPACE METHODS

In this paper we are concerned with the solution of linear systems

$$A\mathbf{x} = \mathbf{b} \tag{13}$$

where $A \in \mathbb{C}^{n\times n}$ is typically full and non-Hermitian, $\mathbf{x}, \mathbf{b} \in \mathbb{C}^n$. We consider three of the most widely used conjugate gradient type methods (viz. CGN, GMRES, Bi-CGSTAB) which fall in the category of Krylov subspace methods; see also Reference 34 for a recent survey of these schemes. We review these methods briefly with emphasis on the convergence criterion and implementation details as appropriate for boundary element systems. Briefly, starting with an initial guess $\mathbf{x}_0$, iterates $\mathbf{x}_i \in \mathbf{x}_0 + K_i(\mathbf{v}_0, B)$ $(i = 1, 2, \ldots)$ are produced such that the residuals $\mathbf{r}_i = \mathbf{b} - A\mathbf{x}_i$ are in some sense small. The Krylov subspace $K_i(\mathbf{v}_0, B)$ is the linear space spanned by the vectors $\{\mathbf{v}_0, B\mathbf{v}_0, \ldots, B^{i-1}\mathbf{v}_0\}$ or equivalently

$$K_i(\mathbf{v}_0, B) = \{\mathbf{w} \mid \mathbf{w} = p_{i-1}(B)\mathbf{v}_0, \;\; p_{i-1} \in \mathscr{P}_{i-1}\}$$

where $\mathscr{P}_{i-1}$ denotes the space of polynomials of degree less than or equal to $i - 1$.

4.1. Conjugate gradient method

The conjugate gradient method was introduced by Hestenes and Stiefel[35] in 1952 for A a symmetric, positive definite matrix. In this case the unique solution of (13) also minimizes the quadratic functional $\mathscr{F}(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}A\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{b}$; see for example Reference 36.

The conjugate gradient method has the following two important properties:

1. The iterates and residuals satisfy minimization properties in the A and A^{-1} norms respectively, e.g.:

$$\|\mathbf{b} - A\mathbf{x}_i\|_{A^{-1}} = \min_{\mathbf{x} \in \mathbf{x}_0 + K_i(\mathbf{r}_0, A)} \|\mathbf{b} - A\mathbf{x}\|_{A^{-1}} \tag{14}$$

2. The iterates and the residuals satisfy three-term recurrences and hence can be computed efficiently.

As a Krylov subspace method the conjugate gradient scheme produces iterates $\mathbf{x}_i \in \mathbf{x}_0 + K_i(\mathbf{r}_0, A)$. That is $\mathbf{x}_i = \mathbf{x}_0 + p_{i-1}(A)\mathbf{r}_0$ from which it follows that $\mathbf{r}_i = \psi_i(A)\mathbf{r}_0$ where $\psi_i \in \mathscr{P}_i$ and $\psi_i(0) = 1$, an *ith residual polynomial*.

The classical CG method can be used for solving non-Hermitian linear systems when applied to the **N**ormal form of the equations. That is, applied either to

$$A^*A\mathbf{x} = A^*\mathbf{b} \tag{15}$$

referred to as CGNR, or to

$$AA^*\mathbf{y} = \mathbf{b} \quad \text{where } \mathbf{x} = A^*\mathbf{y}$$

referred to as CGNE.[34] Application of the classical CG method to (15) produces iterates where $\mathbf{x}_i \in \mathbf{x}_0 + K_i(A^*\mathbf{r}_0, A^*A)$ with the **R**esiduals satisfying

$$\|\mathbf{r}_i\|_2 = \min_{\mathbf{x} \in \mathbf{x}_0 + K_i(A^*\mathbf{r}_0, A^*A)} \|\mathbf{b} - A\mathbf{x}\|_2 \tag{16}$$

For CGNE the minimization property reduces to 2-norm minimization of the *error*.

In this paper we concentrate on the CGNR formulation. It readily follows that

$$\mathbf{r}_i = \psi_i(AA^*)\mathbf{r}_0 \tag{17}$$

The convergence of the method is fast if $\|\psi_i(AA^*)\|$ decays rapidly with i. Since AA^* is a normal matrix, it follows that

$$\|\psi_i(AA^*)\|_2 = \|\psi_i\|_{\Sigma^2} := \max_{s \in \Sigma^2} |\psi_i(s)| \tag{18}$$

Σ denotes the ordered set of singular values of A, i.e. $\sigma_1 \leqslant \sigma_2 \leqslant \cdot\ \cdot\ \cdot \leqslant \sigma_n$ and $\Sigma^2 = \{\sigma_1^2, \sigma_2^2, \ldots, \sigma_n^2\}$, the set of eigenvalues of AA^*. It now follows from (16)–(18) that

$$\frac{\|\mathbf{r}_i\|_2}{\|\mathbf{r}_0\|_2} \leqslant \inf_{\substack{\psi_i \in \mathscr{P}_i \\ \psi_i(0)=1}} \|\psi_i\|_{\Sigma^2} \tag{19}$$

Hence the problem of error analysis of the conjugate gradient method has reduced to minimization of polynomials over a discrete set of real numbers. Choosing as ψ_i, the Chebyshev polynomial T_i suitably shifted to $[\sigma_1^2, \sigma_n^2]$ and normalized such that $T_i(0) = 1$ gives the well-known estimate

$$\frac{\|\mathbf{r}_i\|_2}{\|\mathbf{r}_0\|_2} \leqslant 2\left(\frac{\kappa - 1}{\kappa + 1}\right)^i \tag{20}$$

where $\kappa = \kappa(A) = \sigma_n/\sigma_1$ is the 2-norm condition number of A. Therefore, it follows from (19) that it is the square of the singular values of A which play an important role in the convergence behaviour of CGNR.

The cost per iteration is fixed and dominated by two matrix–vector multiplications. For boundary integral equations where the linear systems are fully populated, the use of any iterative method can only be justified if convergence to within the level of discretization error can be achieved in a small number of iterations compared to n. This is the case when $A \in \mathbb{C}^{n \times n}$ is a matrix representing the discretization of a second kind Fredholm operator $\mathscr{A} = \lambda\mathscr{I} - \mathscr{K}$, where $\mathscr{K}$ is compact. The eigenvalues of $\mathscr{K}$ will typically behave as $\mathscr{O}(n^\alpha)$, where $\alpha \leqslant -1$ is the order of the operator. The smoother the operator $\mathscr{K}$ the faster the eigenvalues of $\mathscr{A}$ hence those of A approach their point of accumulation. Here, the elements of Σ^2 cluster in the vicinity of $|\lambda|^2$, thus from (19) we can expect CGNR to converge in a small number of iterations, see Reference 18.

Like all error bounds involving condition numbers, (20) though informative, is in general over pessimistic. However, it does indicate that the use of CGNR or CGNE is perhaps inappropriate for finite difference or finite element equations, even with preconditioning, since $\kappa(A)$ is typically $\mathcal{O}(n^2)$ for second-order differential equations. On the other hand, in boundary element applications $\kappa(A) = \mathcal{O}(1)$ (e.g. second kind equations) or $\mathcal{O}(n)$ (hypersingular or first kind equations) hence the use of CGN may still prove acceptable. See Appendix II for an outline of the CGNR algorithm.

4.2. GMRES

The Generalized Minimal RESidual (GMRES) method of Saad and Schultz[37] works directly with the non-Hermitian system (13). It is a Krylov subspace method where $\mathbf{x}_i \in \mathbf{x}_0 + K_i(\mathbf{r}_0, A)$. Each iterate is obtained by imposing the minimization condition

$$\|\mathbf{b} - A\mathbf{x}_i\|_2 = \min_{\mathbf{x} \in \mathbf{x}_0 + K_i(\mathbf{r}_0, A)} \|\mathbf{b} - A\mathbf{x}\|_2 \tag{21}$$

Condition (21) is essentially the same as (14) except for the change to the 2-norm as A^{-1} no longer defines an energy norm. The minimization problem (21) always has a unique solution. However, unlike the case of the classical conjugate gradient method, it is not possible to obtain a short recurrence relation between successive iterates. As i increases so does the cost of solving (21) since the number of vectors requiring storage grows linearly. This is related to the underlying Arnoldi process for obtaining an orthogonal basis for Krylov subspaces. In practice it may be necessary and advisable to limit ourselves to storing a maximum of m vectors, and hence restarting GMRES every m iterations, using the last residual as the new initial residual. This scheme is referred to as GMRES(m).

As a Krylov subspace method, it is easy to see that the residuals in the GMRES satisfy

$$\mathbf{r}_i = \psi_i(A)\mathbf{r}_0 \tag{22}$$

where $\psi_i(s)$ is a residual polynomial of degree i satisfying $\psi_i(0) = 1$ for all i. Speed of convergence depends on the size of $\|\psi_i(A)\|$. We can relate this to the properties of the eigensystem of A. If V denotes any matrix of the eigenvectors of A, i.e. $V^{-1}AV = D$, where D is the diagonal matrix of the eigenvalues of A, with the spectrum $\Lambda = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$, then it is easy to show that $V^{-1}\psi_i(A)V = \psi_i(D)$ and hence

$$\|\psi_i(A)\|_2 \leqslant \|V\|_2 \|V^{-1}\|_2 \|\psi_i\|_\Lambda = \kappa(V)\|\psi_i\|_\Lambda. \tag{23}$$

It now follows from (21)–(23) that

$$\frac{\|\mathbf{r}_i\|_2}{\|\mathbf{r}_0\|_2} \leqslant \kappa(V) \inf_{\substack{\psi_i \in \mathcal{P}_i \\ \psi_i(0) = 1}} \|\psi_i\|_\Lambda \tag{24}$$

As the eigenvalues of A may now be complex, elegant error bounds such as (20) cannot be deduced, yet clearly eigenvalue clustering is still a desirable feature of the matrix. If $\kappa(V)$ is large, which happens for eigenvalues which are sensitive to matrix perturbation, then the bounds (23) and (24) are unrealistically pessimistic. For such highly non-normal matrices it is now acknowledged that bounds involving the ε-pseudospectrum of A are more realistic; see References 38 and 39 for more details. In our numerical experiments presented in Section 5, the matrices are 'near' normal with $\kappa(V)$ small or moderate, thus the convergence of GMRES will be

chiefly dependent upon the eigenvalue distribution. See Appendix II for an outline of the GMRES algorithm.

4.3. Bi-CGSTAB

The methods discussed so far have been based on the minimization of the residual in appropriate norms: A^{-1}-norm for the case when A is Hermitian, positive definite, or the 2-norm for CGN and GMRES. For general non-Hermitian systems CGN is the only CG-type method which retains both the minimization and short-term recurrence properties of Section 4.1. Instead of basing our Krylov method on a residual norm minimization process, we can choose to retain the short recurrence relation property. We are then led to a Galerkin-type criterion to be satisfied by the residuals. That is we enforce $\mathbf{r}_i \perp \mathscr{L}_i$, where $\mathscr{L}_i$ is some i-dimensional subspace to be specified below.

The Bi-Conjugate Gradient method[40] is related to the non-symmetric Lanczos tridiagonalization process for finding the eigenvalues of A. The method involves both A and A^*, and uses short recurrences with two sets of vectors. Bi-CG is a Krylov subspace method where $\mathbf{x}_i \in \mathbf{x}_0 + K_i(\mathbf{r}_0, A)$ is obtained such that

$$\mathbf{r}_i \perp K_i(\tilde{\mathbf{r}}_0, A^*)$$

for some other initial vector $\tilde{\mathbf{r}}_0$. It can be shown that $\mathbf{r}_i = \psi_i(A)\mathbf{r}_0$ and $\tilde{\mathbf{r}}_i = \bar{\psi}_i(A^*)\tilde{\mathbf{r}}_0$, where $\bar{\psi}_i$ is the polynomial formed by conjugating the coefficients of ψ_i, thus the above orthogonality criterion implies that

$$\tilde{\mathbf{r}}_i^* \mathbf{r}_j = \gamma_i \delta_{ij}$$

where $\gamma_i \neq 0$ is a constant and δ_{ij} is the Kronecker delta symbol. Therefore, for $i \neq j$

$$0 = \langle \bar{\psi}_i(A^*)\tilde{\mathbf{r}}_0, \psi_j(A)\mathbf{r}_0 \rangle$$

$$= \tilde{\mathbf{r}}_0^* \psi_i(A)\psi_j(A)\mathbf{r}_0$$

From this Sonneveld[41] observed that it is possible to implement a version of the Bi-CG algorithm that only requires A and not A^*. The residuals in Sonneveld's algorithm satisfy $\mathbf{r}_i = \psi_i^2(A)\mathbf{r}_0$, where ψ_i is the Bi-CG polynomial. For this reason his method is referred to Conjugate Gradient Squared (CGS). When Bi-CG converges CGS converges typically twice as fast, though the residuals often have very erratic behaviour. This is clearly undesirable in practice since the size of successive residual norms gives no indication of the proximity to the true solution thus we would have to perform extra, possibly unnecessary, iterations.

In order to smooth the convergence of CGS, Van der Vorst[42] proposed modified iterations where

$$\mathbf{r}_i = \psi_i(A)\phi_i(A)\mathbf{r}_0 \tag{25}$$

and

$$\phi_i(z) = (1 - \omega_1 z)(1 - \omega_2 z)\cdots(1 - \omega_i z)$$

$$= (1 - \omega_i z)\phi_{i-1}(z); \quad \phi_0(z) \equiv 1$$

with the ω_i chosen such that $\|\mathbf{r}_i\|_2$ is minimized over $\omega_i \in \mathbb{C}$.[43] This stabilized version of Bi-CG is referred to as Bi-CGSTAB. See Appendix II for an outline of this algorithm.

As with all Bi-CG methods based upon the unsymmetric Lanczos process, Bi-CGSTAB may suffer breakdown. This occurs when either $\langle \tilde{\mathbf{r}}_0, \mathbf{r}_i \rangle = 0$ or $\langle \tilde{\mathbf{r}}_0, A\mathbf{p}_i \rangle = 0$ but $\mathbf{r}_i \neq 0$. A class of look-ahead Lanczos algorithms have been developed to overcome possible breakdowns; see Reference 36 and references therein. When breakdown does not occur the convergence of Bi-CGSTAB is fast and the residual norm history ($\|\mathbf{r}_i\|$ vs. iteration number) is smooth.

4.4. Preconditioning

In each of the methods considered here the work is dominated by the number of matrix–vector (MV) multiplications performed per iteration. CGNR and Bi-CGSTAB both require two MVs, but the former also requires the conjugate transpose matrix. The GMRES method only needs one MV per iteration but the amount of storage increases at each step. Theoretically, in the absence of rounding errors, CGNR and GMRES converge to the true solution in $\leqslant n$ iterations, see equations (16) and (21). In practice we hope to achieve convergence to the level of discretization error in far fewer than n iterations.

The convergence of these methods is rapid if the matrix has a small condition number (i.e. σ_1 away from zero and σ_n not too large) and its eigenvalues are clustered. If A does not satisfy these conditions then it may be possible to find a preconditioning matrix D such that $D^{-1}A$ has the desired properties. We would then apply our iterative methods to the preconditioned system $D^{-1}A\mathbf{x} = D^{-1}\mathbf{b} = \mathbf{b}'$. Clearly $D \approx A$ is a desirable property for any preconditioner, but we must bear in mind that the solution of linear systems of the form $D\mathbf{w} = \mathbf{t}$ will be required at each iteration corresponding to every MV operation. This restricts the choice of our preconditioner to those which are cheap to invert but still mimic accurately important spectral features of A. See Reference 44 for a discussion of several sparse preconditioners for boundary element systems.

Let us return to our boundary element system $A\mathbf{x} = \mathbf{b}$ which represents the discretization of (10) for the Neumann problem. The matrix A is the discretization of the strongly elliptic pseudodifferential operator $\mathscr{A} = \mathscr{A}_{k,\eta} = -\frac{1}{2}\mathscr{I} + \mathscr{M}_k + i\eta\mathscr{N}_k$ of order $+1$. Strong ellipticity implies the existence of operators $\mathscr{D}$ and $\mathscr{C}$ such that $\mathscr{A} = \mathscr{D} - \mathscr{C}$, where $\mathscr{D}$ is positive (or negative) definite, bounded with bounded inverse and $\mathscr{C}$ is compact; see Reference 4 and references therein. The theoretical advantage of this splitting is that $\mathscr{A}\phi = f$ is equivalent to the second kind Fredholm equation $(\mathscr{I} - \mathscr{D}^{-1}\mathscr{C})\phi = \mathscr{D}^{-1}f$. Motivated by this, we consider splitting A as $A = D - C$ where D denotes the discretization of the most dominant part of $\mathscr{A}_{k,\eta}$, and C is the discretization of the 'smooth' remainder. With this splitting the boundary element system can be rewritten as

$$B\mathbf{x} = \mathbf{b}' \tag{26}$$

where $B = I - D^{-1}C$ with its eigenvalues clustered around 1. The choice of the preconditioner D will now be discussed.

For the boundary integral equations of interest here, governed by the hypersingular operator $\mathscr{N}_k$, each row of the system will be dominated by contributions from the element containing the collocation point and those elements close to the collocation point. For the piecewise constant approximation used here, we take for D the tridiagonal band of A together with the extreme anti-diagonal corner elements $a_{1,n}$ and $a_{n,1}$. We refer to this matrix as Periodic Tridiagonal (PT). This choice of D corresponds to taking the contributions from the element containing the collocation

point and one element on either side of it.[45] For higher-order elements we will take for D an appropriate block periodic tridiagonal part of A.

An important aspect of our PT preconditioner is that it can be LU factorised in $\mathcal{O}(n)$ operations, as is shown explicitly below.

$$D = \mathrm{PT}(A) = \begin{pmatrix} a_{11} & a_{12} & & & a_{1n} \\ a_{21} & a_{22} & a_{23} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & a_{n-1\,n} \\ a_{n1} & & & a_{n\,n-1} & a_{nn} \end{pmatrix}$$

$$= \begin{pmatrix} a_{11} & & & & & & \\ a_{21} & l_2 & & & & & \\ & a_{32} & l_3 & & & & \\ & & \ddots & \ddots & & & \\ & & & \ddots & \ddots & & \\ & & & & a_{n-1\,n-2} & l_{n-1} & \\ a_{n1} & k_2 & \cdots & \cdots & k_{n-2} & k_{n-1} & l_n \end{pmatrix} \begin{pmatrix} 1 & u_1 & & & & & v_1 \\ & 1 & u_2 & & & & v_2 \\ & & \ddots & \ddots & & & \vdots \\ & & & \ddots & \ddots & & \vdots \\ & & & & 1 & u_{n-2} & v_{n-2} \\ & & & & & 1 & u_{n-1} \\ & & & & & & 1 \end{pmatrix}$$

$$= \begin{pmatrix} a_{11} & a_{11}u_1 & & & & & a_{11}v_1 \\ a_{21} & a_{21}u_1 + l_2 & l_2u_2 & & & & a_{21}v_1 + l_2v_2 \\ & a_{32} & a_{32}u_2 + l_3 & l_3u_3 & & & a_{32}v_2 + l_3v_3 \\ & & \ddots & \ddots & \ddots & & \vdots \\ & & & \ddots & a_{n-1\,n-2}u_{n-2} + l_{n-1} & & a_{n-1\,n-2}v_{n-2} + l_{n-1}u_{n-1} \\ a_{n1} & a_{n1}u_1 + k_2 & k_2u_2 + k_3 & \cdots & k_{n-2}u_{n-2} + k_{n-1} & & \begin{cases} a_{n1}v_1 + \sum_{i=2}^{n-2} k_iv_i \\ + k_{n-1}u_{n-1} + l_n \end{cases} \end{pmatrix}$$

To obtain the $4n-6$ unknown coefficients of the matrices L and U, we need to compare systematically the elements of D with the corresponding elements in the product LU. The usual scheme is to find the first *column* of L, by comparing the first column of A with that of the product LU, followed by the first *row* of U, by comparing the first row of A with that of LU and so on. These are found as follows:

$u_1 = a_{12}/a_{11},\ v_1 = a_{1n}/a_{11},\ l_2 = a_{22} - a_{21}u_1,\ k_2 = -a_{n1}u_1,\ s = a_{n1}v_1$
For $i = 2 : n-2$
  $u_i = a_{i\,i+1}/l_i$
  $v_i = -a_{i\,i-1}v_{i-1}/l_i$
  $l_{i+1} = a_{i+1\,i+1} - a_{i+1\,i}u_i$
  $k_{i+1} = -k_iu_i$
  $s = s + k_iv_i$
end
$k_{n-1} = k_{n-1} + a_{n\,n-1}$
$u_{n-1} = (a_{n-1\,n} - a_{n-1\,n-2}v_{n-2})/l_{n-1}$
$l_n = a_{nn} - k_{n-1}u_{n-1} - s$

Elements of L and U are computed once and stored as 4 vectors. Thus to solve $D\mathbf{w}=\mathbf{t}$, we must first solve $L\mathbf{y}=\mathbf{t}$, followed by $U\mathbf{w}=\mathbf{y}$. A simple algorithm for the solution is presented below.

Step 1:

$y_1 = t_1/a_{11}$
$s = a_{n1}y_1$
For $i = 2 : n-1$
  $y_i = (t_i - a_{i\,i-1}y_{i-1})/l_i$
  $s = s + k_i y_i$
end
$y_n = (t_n - s)/l_n$

Step 2:

$w_n = y_n$
$w_{n-1} = y_{n-1} - u_{n-1}w_n$
For $i = n-2 : -1 : 1$
  $w_i = y_i - u_i w_{i+1} - v_i w_n$
end

5. NUMERICAL EXPERIMENTS

For the test problems presented here we take the closed boundary Γ to be either a unit circle centred at the origin, or an ellipse with equation $(x/a)^2 + (y/b)^2 = 1$ of approximate length 2π with minor to major axis ratio 1 : 2 (i.e. $a = 0{\cdot}65,\ b = 1{\cdot}30$). In both cases Γ is divided into equal length elements with collocation points at element midpoints. We consider the surface pressure on Γ due to a point source of unit strength placed at $p^* = (0{\cdot}5, 0{\cdot}0)$, within Γ. The true solution for points $p \in \Gamma$ is given by $\phi(p) = (i/4)H_0^{(1)}(kr)$ where $r = |p^* - p|$ and k is the wave number of the source, see References 1 and 20 for details on this type of test problem. For our numerical results to have a comparable level of accuracy for different values of the wave number, in this section we generally take as the number of collocation points $n = 12k$. In the tables ratio = 1 and 2 refer to the circle and ellipse respectively. We compare the performance of the three Krylov subspace methods introduced in Section 4 and the corresponding PT-preconditioned versions.

The case $\eta = 0$ corresponds to the Surface Helmholtz Equation, equation (6), a second kind Fredholm equation. The eigenvalues of A should cluster about $-\frac{1}{2}$. To demonstrate this effect we plot, in the complex plane, the eigenvalues of A for the representative problem of the unit circle at $k = 8$ with $n = 96$ elements, giving 49 distinct eigenvalues (Figure 1).

The eigenvalues of the operator $\mathcal{N}_k$ are dominated by those of $\mathcal{N}_0$, the corresponding operator for Laplace's equation. It can be shown that on a unit circle

$$\lambda_{\mathcal{N}_0,m} = -m/2 \tag{27}$$

with corresponding eigenfunctions $e^{\pm im\theta}$. Note that (27) agrees with the asymptotic results for $\lambda_{\mathcal{N}_k,m}$ presented in Section 3. Clearly there is no clustering of the eigenvalues of the operators $\mathcal{N}_0$ or $\mathcal{N}_k$. In Appendix I we show that the eigenvalues of the $n \times n$ matrix approximation to $\mathcal{N}_0$ are given by

$$\lambda_\ell = -\frac{n}{2\pi}\sin\left(\frac{\ell\pi}{n}\right), \quad \ell = 0, 1, \ldots, n-1 \tag{28}$$

Note that for $\ell \ll n$, $\lambda_\ell = -\ell/2 + \mathcal{O}(n^{-2})$, agreeing with (27) to within the limitations of the piecewise constant approximation. From (28) it can be seen that the eigenvalues of the discrete operator show a point of accumulation around $-n/2\pi$. The dependence of the cluster point on n indicates that this is not a 'true' clustering, unlike the case for compact operators. The eigenvalues of the discrete approximation of the Burton and Miller operator $\mathcal{A}_{k,\eta} = -\frac{1}{2}\mathcal{I} + \mathcal{M}_k + i\eta\mathcal{N}_k$ cluster

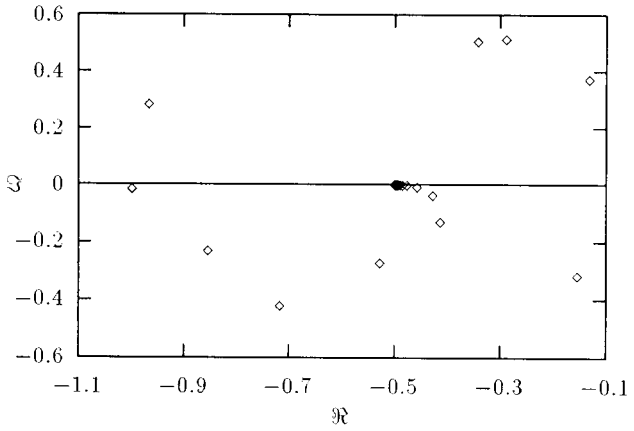

Figure 1. Eigenvalue distribution ($\eta = 0$)

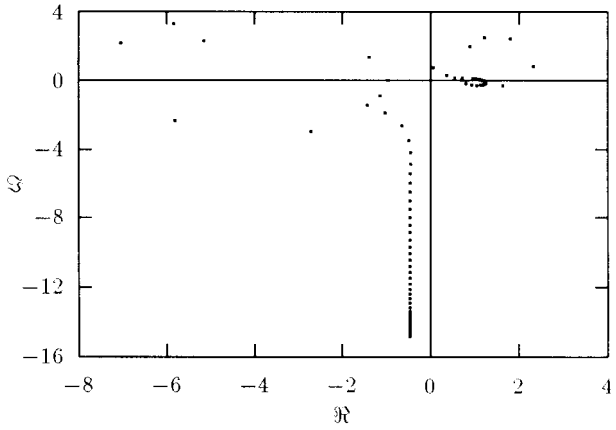

Figure 2. Eigenvalue distribution ($\eta = 1$)

near $-\frac{1}{2} + i\eta\lambda_{n/2}$. This behaviour can be clearly observed from the plots of the eigenvalues of A, corresponding to the case $n = 96$, $k = 8$ with $\eta = 1$ and $\eta = 1/k$, lying in the left half plane of Figures 2 and 3 respectively. Recall that the choice of coupling parameter $\eta = 1/k$ reduces the condition number of the operator $\mathscr{A}_{k,\eta}$ (see Section 3) and this is also reflected in the condition number of the discrete system. For the above problem values of the pseudo-condition number, $\max|\lambda_A|/\min|\lambda_A|$, are 14·85 for the case $\eta = 1$ and 3·76 when $\eta = 1/k$.

The PT-preconditioning has the effect of almost reducing the problem to one of a second kind Fredholm equation. This is demonstrated by the 'true' clustering of the eigenvalues of the preconditioned matrix $D^{-1}A$ about 1. Results are presented for the same problems as above, now the eigenvalues lying on the right half plane in Figures 2 and 3.

In Tables I–III the number of iterations required to achieve accuracy to the level of discretization error are shown for CGNR, Bi-CGSTAB and GMRES, with the corresponding PT-preconditioned versions.

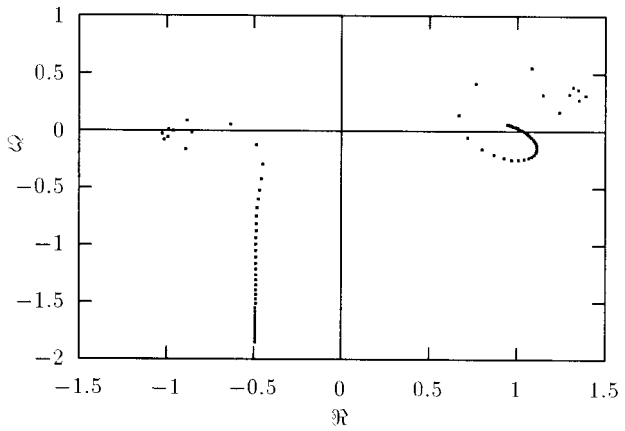

Figure 3. Eigenvalue distribution ($\eta = 1/k$)

Table I. CGNR and PT-CGNR

$k(n)$	Ratio	$\eta = 0$	$\eta = 1$	$\mathrm{PT}_{\eta=1}$	$\eta = 1/k$	$\mathrm{PT}_{\eta=1/k}$
3(36)	1	7	16	5	9	5
	2	9	14	6	11	5
3(72)	1	7	30	6	17	5
	2	10	31	7	21	6
5(60)	1	8	17	6	7	6
	2	10	27	10	14	7
5(120)	1	8	30	9	13	6
	2	10	55	14	31	8
8(96)	1	9	25	10	7	6
	2	11	30	13	14	7
10(120)	1	14	26	12	7	6
	2	14	50	15	12	7

Table II. Bi-CGSTAB and PT-Bi-CGSTAB

$k(n)$	Ratio	$\eta = 0$	$\eta = 1$	$\mathrm{PT}_{\eta=1}$	$\eta = 1/k$	$\mathrm{PT}_{\eta=1/k}$
3(36)	1	6	8	6	8	4
	2	7	9	6	8	4
3(72)	1	6	12	6	10	4
	2	7	12	7	11	5
5(60)	1	7	9	6	6	4
	2	7	11	6	6	4
5(120)	1	8	12	8	8	4
	2	8	15	8	10	5
8(96)	1	9	12	8	4	3
	2	10	15	10	7	3
10(120)	1	10	12	10	4	3
	2	11	17	11	4	3

Table III. GMRES and PT-GMRES

$k(n)$	Ratio	$\eta=0$	$\eta=1$	$\mathrm{PT}_{\eta=1}$	$\eta=1/k$	$\mathrm{PT}_{\eta=1/k}$
3(36)	1	10	24	10	16	9
	2	11	24	12	17	10
3(72)	1	11	44	12	25	10
	2	11	45	13	28	10
5(60)	1	12	23	12	15	10
	2	14	32	14	16	11
5(120)	1	13	55	16	26	12
	2	14	65	18	32	13
8(96)	1	15	53	13	15	10
	2	20	54	15	17	11
10(120)	1	23	52	16	14	9
	2	22	59	17	13	9

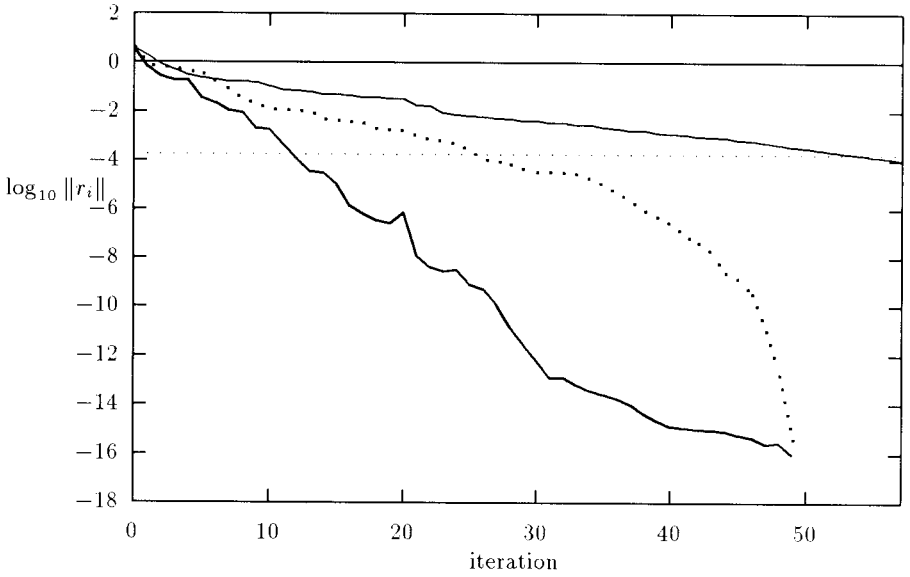

Figure 4. Residual norm history ($\eta=1$)

For the case $\eta=0$ doubling the number of collocation points for k fixed does not lead to a large increase in the number of iterations as expected for a second kind equation. For the Burton and Miller case CGNR and GMRES typically need twice as many iterations as n is doubled due to lack of eigenvalue clustering because of the presence of $\mathcal{N}_k$. The choice $\eta=1/k$ improves the conditioning of the discrete system, hence we require less iterations. The PT-preconditioned versions require far fewer iterations, and increasing the accuracy leads to only a small increase in the number of iterations, demonstrating the second kind behaviour.

Figures 4 and 5 show the residual norm history for the unpreconditioned CGNR (dark dotted line), Bi-CGSTAB (dark solid line) and GMRES (light solid line) for the circle test problem at

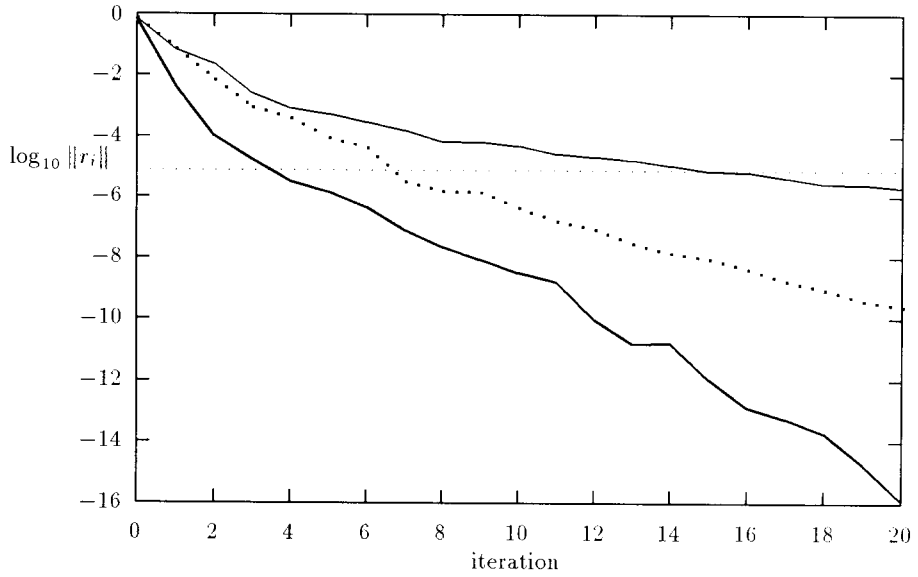

Figure 5. Residual norm history ($\eta = 1/k$)

$k = 8$ with $n = 96$. The horizontal dotted line indicates the level of accuracy at which we would stop, based on the discretization error criterion.

Notice that the convergence of CGNR and GMRES is monotonic ($\|r_{i+1}\| < \|r_i\|$) whereas that of Bi-CGSTAB can have some sharp peaks. Similar plots for CGS, not included here, show much greater jaggedness. It must be borne in mind that GMRES only requires one matrix–vector multiplication per iteration, thus it appears that it can be competitive with CGNR, without the inherent problem of 'squaring the condition number', see Section 4. In all cases Bi-CGSTAB outperforms the other two methods.

6. CONCLUSIONS

In this paper we have studied the efficient solution of boundary element systems arising from the Helmholtz equation by iterative methods from the Krylov subspace class. We have analysed the spectral properties of the Helmholtz operators on a circle from which the asymptotic eigenvalue behaviour were deduced. To tie up with the theoretical results presented in this paper, we considered two simple boundaries where we demonstrated the effectiveness of our efficient *periodic tridiagonal* preconditioner in reducing a hypersingular boundary element discretization to one with clustered eigenvalues, behaving like a second kind Fredholm equation, the ideal situation for the convergence of many iterative methods. Although our preconditioner will work with more complicated boundaries and other boundary integral operators, it is most successful in cases where the essential qualitative features of the boundary element matrix is dominated by the periodic tridiagonal matrix D. We have also shown the influence of the coupling parameter on the condition of the system. We point out that the choice of $\eta = 1/k$ as the *almost optimal* was based on Γ being a circle (or a sphere). For elongated domains or boundaries with corners and edges this

choice of the coupling parameter may not necessarily improve the conditioning. The convergence of both CGNR and GMRES has been shown to be largely dependent upon the eigensystem of the matrix—with eigenvalue clustering a highly desirable feature. The convergence of Bi-CGSTAB is not well understood but we have not encountered breakdown and of the three methods investigated here Bi-CGSTAB is the easiest to implement and in our experience proves the most efficient. Important new results on the eigenvalues of the discrete approximations of the hypersingular operator are presented in Appendix I.

APPENDIX I

The operator $\mathcal{N}_0$ and its matrix approximation

The operator $\mathcal{N}_0$ is defined as for $\mathcal{N}_k$ in (8) with $G_k(p,q)$ replaced by $G_0(p,q) = -(1/2\pi)\ln r$, $r = |p-q|$, the fundamental solution for Laplace's equation. For the spectral analysis of the $\mathcal{N}_k$, it is sufficient to study the properties of $\mathcal{N}_0$, since $\mathcal{N}_k - \mathcal{N}_0$ is compact.

In order to carry out analytical investigation we consider the case where the boundary Γ is a circle of radius a. From the definition

$$(\mathcal{N}_0\phi)(p) = \frac{\partial}{\partial n_p}\int_\Gamma \frac{\partial G_0}{\partial n_q}(p,q)\phi(q)\,\mathrm{d}\Gamma_q = \Xint=_\Gamma \frac{\partial^2 G_0}{\partial n_p \partial n_q}(p,q)\phi(q)\,\mathrm{d}\Gamma_q$$

where the double bar through the integral sign indicates that the integrand is hypersingular with $\mathcal{O}(r^{-2})$ behaviour as $r \to 0$ and the integral should be interpreted and evaluated in the sense of Hadamard's finite part. Points p and q lie on the circle at angles θ_p and θ_q respectively, hence

$$r = |p-q| = 2a\left|\sin\left(\frac{\theta_p - \theta_q}{2}\right)\right|$$

The kernel of the integral may be written as

$$\frac{\partial^2 G_0}{\partial n_p \partial n_q} = \frac{\partial G_0}{\partial r}\frac{\partial^2 r}{\partial n_p \partial n_q} + \frac{\partial^2 G_0}{\partial r^2}\frac{\partial r}{\partial n_p}\frac{\partial r}{\partial n_q}$$

which simplifies to

$$\frac{\partial^2 G_0}{\partial n_p \partial n_q}(r) = \frac{1}{2\pi r^2}$$

Since $\mathrm{d}\Gamma_q = a\,\mathrm{d}\theta_q$ we find that

$$\begin{aligned}(\mathcal{N}_0\phi)(\theta_p) &= \Xint=_0^{2\pi} \frac{a}{2\pi r^2}\phi(\theta_q)\,\mathrm{d}\theta_q \\ &= \frac{1}{8\pi a}\Xint=_0^{2\pi} \operatorname{cosec}^2\left(\frac{\theta_p - \theta_q}{2}\right)\phi(\theta_q)\,\mathrm{d}\theta_q \end{aligned} \tag{29}$$

As for the case of the single and double layer potentials, the eigenfunctions of the operator $\mathcal{N}_0$ are the Fourier modes e^{jmt}, $m \in \mathbb{Z}$. Hence to find the eigenvalues we need to investigate the integral

$$(\mathcal{N}_0 \mathrm{e}^{jm\cdot})(s) = \frac{1}{8\pi a}\Xint=_0^{2\pi} \operatorname{cosec}^2\left(\frac{s-t}{2}\right)\mathrm{e}^{jmt}\,\mathrm{d}t = \frac{1}{8\pi a} I_m$$

The integrals I_m may be calculated by integrating by parts twice, this gives

$$\begin{aligned} I_m &= 2jm \int_0^{2\pi} \cot\left(\frac{s-t}{2}\right) \mathrm{e}^{jmt}\,\mathrm{d}t \\ &= 4m^2 \int_0^{2\pi} \ln\left|\sin\left(\frac{s-t}{2}\right)\right| \mathrm{e}^{jmt}\,\mathrm{d}t \\ &= -4\pi|m|\mathrm{e}^{jms} \end{aligned}$$

where the last line follows from the eigenvalues of the single layer operator; see also Reference 46. Hence

$$(\mathscr{N}_0 \mathrm{e}^{jm\cdot})(s) = -\frac{|m|}{2a}\mathrm{e}^{jms} \tag{30}$$

Suppose $\phi \in \mathscr{L}^2[0, 2\pi]$. If we write ϕ as its Fourier series then (30) implies that we may represent the action of the pseudodifferential operator $\mathscr{N}_0$ in the compact form

$$(\mathscr{N}_0\phi)(t) = -\frac{1}{\sqrt{2\pi}} \sum_{m\in\mathbb{Z}} \frac{|m|}{2a}\,\hat{\phi}_m \mathrm{e}^{jmt} \tag{31}$$

Concentrating on the case of the unit circle we now wish to find the elements and eigenvalues of the piecewise constant collocation matrix $\mathscr{P}_n\mathscr{N}_0 := N \in \mathbb{R}^{n\times n}$. Divide $[0, 2\pi]$ into n equal elements with nodes at $t_i = 2\pi i/n$, $i = 0, 1, \ldots, n$ and collocation points at element midpoints. This matrix is circulant and symmetric and is therefore completely defined by its first row. Hence it suffices to consider a single collocation point, say $s_1 = \pi/n$. Denoting by N_i, the ith element of the first row of N, we have $N_i = (\mathscr{N}_0 v_i)(s_1)$, where v_i is the constant basis function

$$v_i(t) = \begin{cases} 1 & t \in [t_{i-1}, t_i] \\ 0 & \text{otherwise} \end{cases}$$

It follows from (29) that

$$\begin{aligned} N_i &= \frac{1}{8\pi} \int_{t_{i-1}}^{t_i} \mathrm{cosec}^2\left(\frac{s_1 - t}{2}\right)\,\mathrm{d}t \\ &= \frac{1}{4\pi}\left\{\cot\frac{\pi}{2n}(2i-3) - \cot\frac{\pi}{2n}(2i-1)\right\} \end{aligned} \tag{32}$$

We now state and prove an important technical lemma, which we require for the eigenvalues of the N matrix.

Lemma 4. For $i = 1, 2, \ldots, n$

$$\cot\frac{\pi}{2n}(2i-1) - \cot\frac{\pi}{2n}(2i-3) = 2\sum_{m=1}^{n} \sin\left(\frac{m\pi}{n}\right)\cos\left(\frac{2m\pi}{n}(i-1)\right) \tag{33}$$

Proof. The right-hand side of equation (33) can be written as

$$2\sum_{m=1}^{n} \sin\left(\frac{m\pi}{n}\right)\cos\left(\frac{2m\pi}{n}(i-1)\right) = \sum_{m=1}^{n}\left\{\sin\left(\frac{m\pi}{n}(2i-1)\right) - \sin\left(\frac{m\pi}{n}(2i-3)\right)\right\}$$

We require equation (1.342.1) from Gradshteyn and Ryzhik:[47]

$$S = \sum_{m=1}^{n} \sin mx = \sin \frac{(n+1)x}{2} \sin \frac{nx}{2} \operatorname{cosec} \frac{x}{2}$$

The product of sines becomes

$$\sin \frac{(n+1)x}{2} \sin \frac{nx}{2} = \frac{1}{2}\left[\cos \frac{x}{2} - \cos \frac{(2n+1)x}{2}\right]$$

$$= \frac{1}{2}\left[\cos \frac{x}{2} - \cos nx \cos \frac{x}{2} + \sin nx \sin \frac{x}{2}\right]$$

and hence

$$S = \frac{1}{2}\left[\cot \frac{x}{2}\{1 - \cos nx\} + \sin nx\right] \tag{34}$$

Setting $x = (\pi/n)(2i - r)$ with $r = 1$ or 3, and since $\sin nx = 0$, $\cos nx = -1$, we find that

$$S = \sum_{m=1}^{n} \sin\left(\frac{m\pi}{n}(2i - r)\right) = \cot \frac{\pi}{2n}(2i - r)$$

which implies equation (33). □

Using the result (33) we obtain an alternative expression for the elements of the matrix N in the form

$$N_i = -\frac{1}{2\pi} \sum_{m=1}^{n} \sin\left(\frac{m\pi}{n}\right) \cos\left(\frac{2m\pi}{n}(i-1)\right) \tag{35}$$

If we now denote by $\mathbf{v}$ the first row of N and define $\mathbf{w}_\ell = (1\ t_\ell\ t_\ell^2 \cdots t_\ell^{n-1})^{\mathrm{T}}$ where $t_\ell = \mathrm{e}^{2j\ell\pi/n}$ for $\ell = 0, 1, \ldots, n-1$ (an nth root of unity), then the eigenvalues of the circulant matrix N are given by the dot products $\mathbf{v}.\mathbf{w}_\ell$.[48] That is

$$\lambda_\ell = \sum_{i=1}^{n} N_i t_\ell^{i-1} = -\frac{1}{2\pi} \sum_{m=1}^{n-1} \sin\left(\frac{m\pi}{n}\right) \sum_{i=1}^{n} \cos\left(\frac{2m\pi}{n}(i-1)\right) t_\ell^{i-1}, \quad \ell = 0, \ldots, n-1 \tag{36}$$

To simplify the above expression we need a further technical lemma.

Lemma 5.

$$\sum_{i=1}^{n} \cos\left(\frac{2m\pi}{n}(i-1)\right) t_\ell^{i-1} = \begin{cases} \frac{n}{2} & m = \ell \text{ or } m = n - \ell \\ 0 & \text{otherwise} \end{cases}$$

Proof. The summation may be written

$$2\sum_{i=1}^{n} \cos\left(\frac{2m\pi}{n}(i-1)\right) t_\ell^{i-1} = \sum_{i=1}^{n} (\mathrm{e}^{(2jm\pi/n)(i-1)} + \mathrm{e}^{-(2jm\pi/n)(i-1)})\mathrm{e}^{(2j\ell\pi/n)(i-1)}$$

$$= \sum_{i=1}^{n} \{\mathrm{e}^{(2j\pi/n)(i-1)(m+\ell)} + \mathrm{e}^{(2j\pi/n)(i-1)(\ell-m)}\}$$

$$= \Sigma_1 + \Sigma_2$$

If $m = n - \ell$ then $\Sigma_1 = n$, otherwise

$$\Sigma_1 = \frac{1 - e^{2\pi j(m+\ell)}}{1 - e^{(2j\pi/n)(m+\ell)}} = 0$$

Similarly if $m = \ell$ then $\Sigma_2 = n$, otherwise

$$\Sigma_2 = \frac{1 - e^{2\pi j(\ell-m)}}{1 - e^{(2j\pi/n)(\ell-m)}} = 0$$

Therefore

$$\sum_{i=1}^{n} \cos\left(\frac{2m\pi}{n}(i-1)\right) t_\ell^{i-1} = \begin{cases} \frac{n}{2} & m = \ell \text{ or } m = n - \ell \\ 0 & \text{otherwise} \end{cases}$$

We note that for $\ell = 0$

$$\sum_{i=1}^{n} \cos\left(\frac{2m\pi}{n}(i-1)\right) t_\ell^{i-1} = \sum_{i=1}^{n} \cos\left(\frac{2m\pi}{n}(i-1)\right) = \begin{cases} n & m = 0 \text{ or } m = n \\ 0 & \text{otherwise} \end{cases}$$

and since $1 \leqslant m \leqslant n-1$, $\lambda_0 = 0$. □

Returning to equation (36) it follows that

$$\lambda_\ell = -\frac{1}{2\pi}\left(\frac{n}{2}\right)\left\{\sin\left(\frac{\ell\pi}{n}\right) + \sin\left(\frac{(n-\ell)\pi}{n}\right)\right\}$$

$$= -\frac{n}{2\pi}\sin\left(\frac{\ell\pi}{n}\right) \quad \ell = 0, 1, \ldots, n-1$$

Note that for $\ell \ll n$, $\lambda_\ell = -\ell/2 + \mathcal{O}(n^{-2})$ agreeing with (30) to within the limitations of the piecewise constant approximation. Since $\lambda_\ell = \lambda_{n-\ell}$ for $\ell = 1, \ldots, \ell_{\max}$ (where $\ell_{\max} = n/2 - 1$ if n is even; $\ell_{\max} = (n-1)/2$, n odd) the eigenvalues occur in pairs, except for the simple eigenvalues $\lambda_{n/2}$ when n is even and $\lambda_0 = 0$. We note that unlike the case of the continuous operator $\mathcal{N}_0$, the eigenvalues λ_ℓ of the matrix N demonstrate a kind of clustering, around $-n/2\pi$, for ℓ close to $n/2$.

APPENDIX II

Algorithms for CGN, GMRES and Bi-CGSTAB

Here we present a brief outline of the three algorithms which we have used in this paper. Details of stopping criteria are not included.

CGNR

Choose $\mathbf{x}_0$ and calculate $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$.
$\mathbf{p}_0 = 0$, $\beta_0 = 0$

Begin Iteration

$$\begin{aligned} \mathbf{p}_i &= A^*\mathbf{r}_{i-1} + \beta_{i-1}\mathbf{p}_{i-1} \\ \alpha &= \|A^*\mathbf{r}_{i-1}\|^2 / \|A\mathbf{p}_i\|^2 \\ \mathbf{x}_i &= \mathbf{x}_{i-1} + \alpha\mathbf{p}_i \end{aligned}$$

$\mathbf{r}_i = \mathbf{r}_{i-1} - \alpha A\mathbf{p}_i$
$\beta_i = \|A^*\mathbf{r}_i\|^2/\|A^*\mathbf{r}_{i-1}\|^2$
End Iteration

GMRES
Choose $\mathbf{x}_0$ and calculate $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$.
$\beta = \|\mathbf{r}_0\|,\ \mathbf{v}_1 = \mathbf{r}_0/\beta$

Begin Iteration
$h_{ji} = \langle A\mathbf{v}_i, \mathbf{v}_j\rangle \quad j = 1, 2, \ldots, i$
$\tilde{\mathbf{v}}_{i+1} = A\mathbf{v}_i - \sum_{j=1}^{i} h_{ji}\mathbf{v}_j$
$h_{i+1\,i} = \|\tilde{\mathbf{v}}_{i+1}\|$
$\mathbf{v}_{i+1} = \tilde{\mathbf{v}}_{i+1}/h_{i+1\,i}$
$\mathbf{x}_i = \mathbf{x}_0 + V_i\mathbf{y}_i$ where $\mathbf{y}_i$ minimises
$\|\beta\mathbf{e}_1 - H_i^{(e)}\mathbf{y}\|_2$
End Iteration.

$\mathbf{e}_1$ is the first column of the $i+1$ identity matrix. V_i is the $n \times i$ matrix with column vectors $\mathbf{v}_1, \ldots, \mathbf{v}_i$ and $H_i^{(e)}$ represents the $(i+1) \times i$ upper Hessenberg full rank matrix of the form

$$H_i^{(e)} = \begin{pmatrix} h_{11} & h_{12} & \cdots & h_{1i} \\ h_{21} & \ddots & & \vdots \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & h_{i\,i-1} & h_{ii} \\ 0 & \cdots & 0 & h_{i+1\,i} \end{pmatrix}$$

See Saad and Schultz[37] for more detail.

Bi-CGSTAB
Choose $\mathbf{x}_0$ and calculate $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$
$\mathbf{p}_0 = \mathbf{v}_0 = 0,\ \tilde{\mathbf{r}}_0 = \mathbf{r}_0$
$\rho_0 = \alpha = \omega_0 = 1$

Begin iteration
$\rho_i = \langle\tilde{\mathbf{r}}_0, \mathbf{r}_{i-1}\rangle$
$\beta = (\rho_i/\rho_{i-1})(\alpha/\omega_{i-1})$
$\mathbf{p}_i = \mathbf{r}_{i-1} + \beta(\mathbf{p}_{i-1} - \omega_{i-1}A\mathbf{p}_{i-1})$
$\alpha = \rho_i/\langle\tilde{\mathbf{r}}_0, A\mathbf{p}_i\rangle$
$\mathbf{s} = \mathbf{r}_{i-1} - \alpha A\mathbf{p}_i$
$\omega_i = \langle A\mathbf{s}, \mathbf{s}\rangle/\|A\mathbf{s}\|^2$
$\mathbf{x}_i = \mathbf{x}_{i-1} + \alpha\mathbf{p}_i + \omega_i\mathbf{s}$
$\mathbf{r}_i = \mathbf{s} - \omega_i A\mathbf{s}$
End Iteration.

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