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PRECONDITIONING METHODS FOR THIN SCATTERING STRUCTURES BASED ON ASYMPTOTIC RESULTS*

JOSEF A. SIFUENTES[†] AND SHARI MOSKOW[‡]

Abstract. We present a method to precondition the discretized Lippmann–Schwinger integral equations to model scattering of time-harmonic acoustic waves through a thin inhomogeneous scattering medium. The preconditioner is based on asymptotic results as the thickness of the third component direction goes to zero and requires solving a two dimensional formulation of the problem at the preconditioning step.

Key words. preconditioner, Helmholtz equation, integral methods, acoustic scattering

AMS subject classifications. 65F08, 65F10, 15A18, 47A10, 47A55

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1. Introduction. We consider the problem of scattering time-harmonic acoustic waves through thin, three dimensional inhomogeneities. This physical phenomenon is relevant in the study of photonic band gap structures. Such structures are designed to guide the propogation of light by blocking certain wavelengths in the band gap, while allowing others to pass freely through. Such structures facilitate information propagation in optical communication networks and in optical computing. We consider three dimensional slab waveguides with two dimensional photonic crystal structure. Such structures are typically constucted with a high refraction index and are imbedded in a homogenous scattering medium, typically air. See [19, 20, 6] for more on thin photonic band gap structures.

We are considering time-harmonic wave phenomenon modeled by the Helmholtz equation, whose solution gives the spatial component of the total wave velocity potential. We solve the Helmholtz equation by numerically approximating the equivalent Lippmann–Schwinger volume integral equation [5]. The resulting finite dimensional linear system is large, dense, and non-Hermitian, but there are efficient matrixvector product routines that make an iterative solver an appealing approach; see, e.g., [1, 3, 8, 7, 14, 15]. However, spectral properties of the system often cause Krylov subspace based iterative methods to converge slowly.

Moskow, Santosa, and Zhang demonstrated in [13] an asymptotic expansion of the Lippmann–Schwinger integral equation for inhomogeneities that are thin in one component direction. They showed that the difference in the solution to a two dimensional integral equation and the full three dimensional problem differed by $\mathcal{O}(h)$ as $h \to 0$, where h is the width of the inhomogeneity in the thin component direction. A natural extension of their work is to precondition the three dimensional problem using the two dimensional operator. In order for this approach to work, one must be able to

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formulate the preconditioner so that it can be applied to three dimensional data and yet be solved with the complexity of a two dimensional problem. We give a solution to this problem in section 2 and describe the numerical implemention in section 4. Furthermore we extend the asymptotic results of [13] into bounds on the GMRES residual applied to the preconditioned system in section 3. In section 5, we demonstrate the effectiveness of the preconditioner to significantly improve convergence speed and the efficacy of the bounds we develop.

1.1. Problem formulation. We consider the setting of an inhomogenous scattering medium $S \in \mathbb{R}^3$, thin in the third component direction, and set in a homogenous host medium such as air or some fluid. Let S be the Cartesian cross product of its two dimensional cross section, Ω and the thin, third component direction [-h/2, h/2], i.e., $S = \Omega \times [-h/2, h/2]$.

The total scattered field $u \in C^2(\mathbb{R}^3)$ is modeled by the Helmholtz equation

(1)
$$\Delta u + \kappa^2 \epsilon(\mathbf{s})u = 0$$
 for all $\mathbf{s} \in \mathbb{R}^3$,

where the parameter κ is called the wave number and defined to be $\kappa = \omega/c_0$ for temporal frequency ω with c_0 denoting the speed of wave propogation in the host medium. The total scattered field $u = u^i + u^s$ is the sum of a given incident wave u^i and a scattered wave u^s . We require the scattered wave to satisfy the Sommerfeld radiation condition, which implies there is no wave reflection at infinity [5]:

(2)
$$\frac{\partial u^s}{\partial r} - i\kappa u^s = o(1/r), \qquad r = \|\mathbf{s}\|$$

The incident wave u^i satisfies the freespace Helmholtz equation, $\Delta u^i + \kappa^2 u^i = 0$ for all of \mathbb{R}^3 .

Since we are considering the setting of two dimensional photonoic crystal structures in a three dimensional scattering inhomogeneity, the refractive index is constant in the direction of the thin component direction. We adapt the convention of Moskow, Santosa, and Zhang [13], where we write that the refractive index is represented by $\epsilon_0(\mathbf{x})/h$, where h is the length of the thin side. While refractive indices are material properties that do not depend on size, high refraction indices are necessary to sufficiently reduce the wavelength on the order of the length of the waveguide in the thin direction. Thus we define the refractive index function

(3)
$$\epsilon(\mathbf{x}, z) = \begin{cases} 1 & \text{for } (\mathbf{x}, z) \notin S; \\ \frac{\epsilon_0(\mathbf{x})}{h} & \text{for } (\mathbf{x}, z) \in S, \end{cases}$$

where ϵ_0 is compactly supported on Ω . If $u = u^s + u^i$ satisfies (1) and (2), then u is also a solution to the Lippmann–Schwinger volume integral equation [5]

(4)
$$u(\mathbf{s}) + \kappa^2 \int_S \left(1 - \frac{\epsilon_o(\mathbf{x}')}{h}\right) G(\mathbf{s}, \mathbf{s}') u(\mathbf{s}') \, d\mathbf{s}' = u^i(\mathbf{s})$$

where \mathbf{x}' is the vector of the first two components of \mathbf{s}' and $G(\mathbf{s})$ is the freespace Green's function given by

(5)
$$G(\mathbf{s}, \mathbf{s}') = \frac{e^{i\kappa \|\mathbf{s}-\mathbf{s}'\|}}{4\pi \|\mathbf{s}-\mathbf{s}'\|}.$$

Separating the integral domain S into Ω and [-h/2, h/2] and letting $s = (\mathbf{x}, z)$ for $\mathbf{x} \in \Omega$ and $z \in [-h/2, h/2]$, we rewrite the Lippmann–Schwinger equation (4) as

$$u(\mathbf{x},z) + \kappa^2 \int_{\Omega} \int_{-h/2}^{h/2} \left(1 - \frac{\epsilon_o(\mathbf{x}')}{h} \right) G((\mathbf{x},z), (\mathbf{x}',z')) u(\mathbf{x}',z') \, dz' d\mathbf{x}' = u^i(\mathbf{x},z),$$

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and apply the linear change of variable $z = h\zeta$ to obtain

$$u(\mathbf{x},\zeta) + \kappa^2 \int_{\Omega} \int_{-1/2}^{1/2} (h - \epsilon_o(\mathbf{x}')) G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta')) u(\mathbf{x}',\zeta') \, dz' d\mathbf{x}' = u^i(\mathbf{x},h\zeta).$$

We write this compactly as

(6)
$$(I+K)u(\mathbf{x},\zeta) = u^{i}(\mathbf{x},h\zeta),$$

where

(7)
$$(Ku)(\mathbf{x},\zeta) := \kappa^2 \int_{\Omega} \int_{-1/2}^{1/2} (h - \epsilon_o(\mathbf{x}')) G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta')) u(\mathbf{x}',\zeta') \, d\zeta' d\mathbf{x}'.$$

2. Application of the GMRES iterative method. Consider applying the GMRES iterative method [16] to the continuous equation (6). Since the operator we are interested in is of the form A := I + K, where K is compact, then A is bounded and has only a finite spectrum outside any neighborhood of one [11, p. 421]. Thus, unlike discretizations of the Helmholtz equation (1), refining the discretizations of the Lippmann–Scwinger equation has little effect on the conditioning of the resulting linear system and therefore little effect on GMRES performance [10, 9]. Numerical experiments in [17] show that increased mesh resolution only adds high frequency eigenmodes to the spectrum, corresponding to eigenvalues of A close to one. Then we should expect that convergence analysis of the continuous case gives insight into convergence behavior of the discretized problem; see, e.g., [2, 12, 18, 21].

The continuous GMRES problem is the iterative minimization problem that solves at iteration m

(8)
$$||r_m|| = \min_{u \in \mathcal{K}_m(A, u^i)} ||u^i - Au||,$$

where $\mathcal{K}_m(A, u^i) := \operatorname{span}\{u^i, Au^i, A^2u^i, \ldots, A^{m-1}u^i\}$ is the Krylov subspace and $\|\cdot\|$ is an appropriate operator norm. In our paper, and following the results of Moskow, Santosa, and Zhang [13], we will use the $L^{\infty}(X)$ vector norm and the operator norm it induces, where X is a compact set in \mathbb{R}^2 or \mathbb{R}^3 depending on context. Since the GMRES solution to the iterative minimization problem is the product of a linear combination of monomials of A and u^i , we can write u_m as a product of a polynomial evaluated at A of degree m-1 and the incident wave u^i , and thus we can write the residual $r_m = u^i - Au_m$ as the product of a polynomial evaluated at A of degree m times u^i , such that the polynomial is one at the origin. Then (8) is equivalent to

$$||r_m|| = \min_{p_m \in \mathcal{P}_m^0} ||p_m(A)u^i||,$$

where \mathcal{P}_m^0 is the set of all polynomials of degree *m* or less with a value of 1 when evaluated at the origin.

In practice, when the GMRES method is applied to the discretized linear system, an orthogonal basis for the approximating space is generated by the Arnoldi iteration [16], and therefore the cost per iteration and memory requirements grows with each iteration as more memory is needed to record the basis for the growing Krylov subspace. Thus, GMRES is feasible if the number of iterations remains small. However GMRES is too computationally expensive for this problem without effective preconditioning. This is where we utilize the asymptotic results of [13] as a guide to building an effective preconditioning scheme. That is, rather than applying GMRES to (6), we solve the equivalent problem

$$\left(AA_0^{-1}\right)\left(A_0u\right) = u^i,$$

where a substantially lower order polynomial in P_m^0 is small when evaluated at AA_0^{-1} , and one can solve $A_0y = z$ relatively quickly for an arbitrary function $z \in C(\overline{S})$. In this case, the right-hand side data need have no physical meaning. (It is actually a basis vector of the Krylov subspace of the current GMRES iteration.) We point out that the regime for which preconditioning is necessary is when $\kappa^2(h-\varepsilon_0)$ is of sufficient magnitude that the compact integral operator K defined in (7) is not less than one in magnitude. Since the operator A is a compact (and thus bounded) perturbation to the identity, if the compact perturbation is relatively small, then GMRES is expected to converge quickly without preconditioning.

To build our preconditioning operator A_0 , consider the two dimensional integral equation

(9)
$$(I - K_{2D})u_0(\mathbf{x}) = u^i(\mathbf{x}, 0),$$

where

(10)
$$(K_{2D}u_0)(\mathbf{x}) := \kappa^2 \int_{\Omega} \epsilon_o(\mathbf{x}') G((\mathbf{x},0),(\mathbf{x}',0)) u_0(\mathbf{x}') \, d\mathbf{x}'.$$

This is the two dimensional operator used to describe asymptotic behavior of a scattered wave over thin scattering domains. Note, however, that in order to use (9) as a preconditioner, we must pose it as a three dimensional integral operator to match the dimensions of the objective problem. Thus we define $K_0: C(\overline{S}) \to C(\Omega)$ by

(11)
$$(K_0 u)(\mathbf{x}, \eta) = K_{2D} \left(\int_{-1/2}^{1/2} u(\mathbf{x}, \eta) \, d\eta \right).$$

Note that K_0 has a domain of continuous functions defined over the three dimensional compact set \overline{S} , but has a range of functions that are constant in the z direction. Then the preconditioning operator is defined to be $A_0 := I - K_0$. Lemma 2 of [13] shows that A_0 is continuously invertible on both $L^2(\overline{S})$ and $C(\overline{S})$.

2.1. Solving the preconditioning step as a two dimensional system. As mentioned before, the right-hand side data for the preconditioning operator A_0 has no physical interpretation, nor is it necessarily constant in the direction of the third component. Furthermore, for such a system $(A_0y)(s) = z(s)$, the solution y(s) need not be constant in the third component direction. However, this preconditioner is only useful if we can solve it as a two dimensional problem.

We solve this problem by noting that if $(A_0y)(s) = z(s)$, then

$$(K_0 y)(\mathbf{s}) = y(\mathbf{s}) - z(\mathbf{s}).$$

This implies that $y(\mathbf{s}) - z(\mathbf{s})$ is constant in the z direction and therefore equal to $\int_{-1/2}^{1/2} y(\mathbf{x},\zeta) - z(\mathbf{x},\zeta) d\zeta$. This gives us the equation

$$\kappa^2 \int_{\Omega} \int_{-1/2}^{1/2} \epsilon(\mathbf{x}') G((\mathbf{x},0),(\mathbf{x}',0)) y(\mathbf{x}',\zeta') \, d\zeta' \, d\mathbf{x}' = \int_{-1/2}^{1/2} y(\mathbf{x},\zeta') - z(\mathbf{x},\zeta') \, d\zeta',$$

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B1010

which can be rearranged to be

$$\begin{split} \int_{-1/2}^{1/2} y(\mathbf{x},\zeta') \, d\zeta' &- \kappa^2 \int_{\Omega} \epsilon(\mathbf{x}') G((\mathbf{x},0),(\mathbf{x}',0)) \left(\int_{-1/2}^{1/2} y(\mathbf{x}',\zeta') \, d\zeta' \right) d\mathbf{x}' \\ &= \int_{-1/2}^{1/2} z(\mathbf{x},\zeta') \, d\zeta \end{split}$$

Define

$$y_a(\mathbf{x}) = \int_{-1/2}^{1/2} y(\mathbf{x}, \zeta') \, d\zeta',$$

$$z_a(\mathbf{x}) = \int_{-1/2}^{1/2} z(\mathbf{x}, \zeta') \, d\zeta'.$$

Then the preconditioning step is equivalent to solving the two dimensional integral equation

$$y_a(\mathbf{x}) - \kappa^2 \int_{\Omega} \epsilon(\mathbf{x}') G((\mathbf{x}, 0), (\mathbf{x}', 0)) y_a(\mathbf{x}') \, d\mathbf{x}' = z_a(\mathbf{x}).$$

Given our solution $y_a(\mathbf{x})$ to the above, we construct our sought after solution by

$$y(\mathbf{x},\zeta) = \kappa^2 \int_{\Omega} \epsilon(\mathbf{x}') G((\mathbf{x},0),(\mathbf{x}',0)) y_a(\mathbf{x}') \, d\mathbf{x}' + z(\mathbf{x},\zeta)$$
$$= y_a(\mathbf{x}) - z_a(\mathbf{x}) + z(\mathbf{x},\zeta).$$

3. Asymptotic results. We present here the main result from Moskow, Santosa, and Zhang [13] and extend it to obtain GMRES convergence bounds when applied to (9) and (10).

THEOREM 1. There exists a constant C, independent of the scattering obstacle thickness h, such that

$$\sup_{(\mathbf{x},\zeta)\in\overline{S}}\int_{\Omega}|G((\mathbf{x},0),(\mathbf{x}',0))-G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))|\ d\mathbf{x}' < Ch.$$

Proof. See Moskow, Santosa, and Zhang [13, Lemma 1].

It follows from [13, Lemma 1] that the constant $C = \kappa M + 1$, and $M = \sup_{\mathbf{x}\in\Omega}\int_{\Omega} \|\mathbf{x} - \mathbf{x}'\|^{-1} d\mathbf{x}'$. We can bound $M \leq \pi d$, where $d = \operatorname{diam}(\Omega)$. This will prove to be useful in computing convergence estimates for the preconditioned scattering problem.

COROLLARY 2. Let A = I + K, where the operator K is defined in (7) and $A_0 = I - K_0$, where K_0 is defined in (11). There exists a constant C', independent of h, but depending on κ such that

$$\left\| I - AA_0^{-1} \right\|_{L^{\infty}(\overline{S})} < C'h.$$

Proof.

$$||I - AA_0^{-1}|| = ||(A_0 - A)A_0^{-1}|| \leq ||A_0^{-1}|| \, ||A_0 - A||.$$

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FIG. 1. Here we illustrate numerically the results of Corollary 2, that $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\| = \mathcal{O}(h)$ (for $\epsilon_0 = 1$). The horizontal dashed line is at 1 and the sloped dashed line is h.

Note that $||A_0^{-1}||$ is independent of h. Consider then the asymptotic term $||A_0 - A||$.

$$\begin{split} \|A - A_0\| \\ &= \sup_{\|\|u\|=1} \|A_0 u - Au\| \\ &= \sup_{\|\|u\|=1} \|K_o u + Ku\| \\ &\leq \sup_{\|\|u\|=1} \sup_{(\mathbf{x},\zeta)\in\overline{S}} \left(h\kappa^2 \int_{-1/2}^{1/2} \int_{\Omega} |G((\mathbf{x},0),(\mathbf{x}',0))| \, |u(s')| \, ds' \\ &+ h\kappa^2 \int_{-1/2}^{1/2} \int_{\Omega} |G((\mathbf{x},0),(\mathbf{x}',0)) - G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))| \\ &\quad |u(\mathbf{x}',\zeta')| \, d\zeta' d\mathbf{x}' \\ &+ \kappa^2 \int_{-1/2}^{1/2} \int_{\Omega} \epsilon_0(\mathbf{x}') \, |G((\mathbf{x},0),(\mathbf{x}',0)) - G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))| \\ &\quad |u(\mathbf{x}',\zeta')| \, d\zeta' d\mathbf{x}' \\ &\quad |u(\mathbf{x}',\zeta')| \, d\zeta' d\mathbf{x}' \\ &\leq h\kappa^2 \left(\frac{M}{4\pi} + Ch + C \|\epsilon_0\|_{L^{\infty}(\Omega)}\right). \end{split}$$

Therefore $||I - AA_0^{-1}||$ is small if the scattering medium is sufficiently thin. However, note that this bound contains the constant $||A_0^{-1}||$, which, while independent of h, could possibly be very large. However, in practice we see that $||I - AA_0||$ is much smaller than the bounds we demonstrate in this corollary, where A and A_0 are discretizations of A and A_0 , respectively, using a collocation method we describe in section 4. We show this in Figure 1.

Π

The reason we do better is that by factoring out the inverse of the preconditioning operator A_0 , we don't take into account spectral deflating. That is, we show in Corollary 3 that $\sigma(A) \in \sigma_{\epsilon}(A_0)$ for $\epsilon = O(h)$. Thus the spectrum of A_0 approximates the spectrum of A. Then the intuition we gain from the numerical results in Figure 1 lead us to believe that we not only approximate well the eigenvalues but also those

B1012



FIG. 2. The spectrum $\sigma(\mathbf{AA}_0^{-1})$ for values of $h = 10^{-1}, 10^{-1.2}, 10^{-1.4}, 10^{-1.6}$ going left to right, top to bottom.

eigenmodes with low enough frequency that they have small dependence on the thin direction component. (Of course the eigenfunctions of A_0 are constant in the thin direction.) Indeed we show that $\sigma(\mathbf{AA}_0^{-1}) \to 1$ as $h \to 0$ in Figure 2.

COROLLARY 3. Let A = I + K, where the operator K is defined in (7), and $A_0 = I - K_0$, where K_0 is defined in (11), then $\sigma(A) \in \sigma_{\epsilon}(A_0)$, where $\epsilon = O(h)$.

Proof. Let (λ, v_0) be an eigenpair of A_0 , such that $||v_0||_{L^{\infty}(\Omega)} = 1$. Then

$$\begin{split} \| (\lambda - A)v_0 \|_{L^{\infty}(\overline{S})} &= \left| \sup_{(\mathbf{x},\zeta)\in\overline{S}} \kappa^2 h \int_{\overline{S}} G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))v_0(\mathbf{x}') \, d\zeta' d\mathbf{x}' \\ &+ \kappa^2 \int_{\Omega} \int_{-1/2}^{1/2} \epsilon_0(\mathbf{x}') \left(G((\mathbf{x},0),(\mathbf{x}',0)) - G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta')) \right) v_0(\mathbf{x}') \, d\zeta' d\mathbf{x}' \right| \\ &\leq h \sup_{(\mathbf{x},\zeta)\in\overline{S}} \left| \kappa^2 \int_{\overline{S}} G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))v_0(\mathbf{x}') \, d\zeta' d\mathbf{x}' \right| \\ &+ \sup_{(\mathbf{x},\zeta)\in\overline{S}} \kappa^2 \int_{\Omega} |\epsilon_0(\mathbf{x}')| \, |v_0(\mathbf{x}')| \int_{-1/2}^{1/2} |G((\mathbf{x},0),(\mathbf{x}',0)) - G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))| \, d\zeta' d\mathbf{x}' \\ &\leq h \| K(\epsilon_0 = 1) \|_{L^{\infty}(\overline{S})} + Ch \| \epsilon_0 \|_{L^{\infty}(\Omega)}, \end{split}$$

where C is the constant from Theorem 1.

Now we can develop a bound for the preconditioned GMRES scheme.

COROLLARY 4. Let A = I + K, where the operator K is defined in (7), and $A_0 = I - K_0$, where K_0 is defined in (11). Then the relative residual of the GMRES problem applied to the right preconditioned problem

$$\left(AA_0^{-1}\right)\left(A_0u\right) = u^i$$

is bounded by ϵ^m at each iteration m, where $\epsilon = O(h)$.

Proof. Recall that we can bound the GMRES residual by the minimal polynomial evaluated at AA_0^{-1} , and that is one at the origin. That is,

$$||r_m|| \le \min_{p_m \in \mathcal{P}_m^0} ||p_m(A)|| ||u^i||.$$

Then Corollary 2 implies that

$$\frac{\|r_m\|}{\|u^i\|} \le \left\| \left(I - AA_0^{-1} \right)^m \right\|$$
$$\le \left\| I - AA_0^{-1} \right\|^m$$
$$\le \epsilon^m,$$

where $\epsilon = O(h)$.

4. Numerical implementation. To facilitate notation of functions on the rescaled slab $\overline{S} := \Omega \times [-1/2, 1/2]$, we use $\overline{f} : \overline{S} \to \mathbb{C}$ to mean that, for $\mathbf{s} \equiv (\mathbf{x}, \zeta) \in \overline{S}$ and f defined on $S = \Omega \times [-h/2, h/2]$, then $\overline{f}(\mathbf{s}) := \overline{f}((\mathbf{x}, \zeta)) := f((\mathbf{x}, h\zeta))$. For example,

$$\bar{G}(\mathbf{s},\mathbf{s}') := \bar{G}((\mathbf{x},\zeta),(\mathbf{x},\zeta)') := G((\mathbf{x},h\zeta),(\mathbf{x},h\zeta)'),
\bar{u}^i(\mathbf{s}) := \bar{u}^i((\mathbf{x},\zeta)) := u^i((\mathbf{x},h\zeta)).$$

We use $f_0: \overline{S} \to \mathbb{C}$ to denote functions that are constant in the z direction, that is, if $f: \overline{S} \to \mathbb{C}$, then $f_0(\mathbf{s}) := f(\mathbf{x}, 0)$. Then, for example,

$$G_0(\mathbf{s}, \mathbf{s}') := G((\mathbf{x}, 0), (\mathbf{x}', 0)),$$

$$u_0^i(\mathbf{s}) := u^i((\mathbf{x}, 0)).$$

We discretize our shifted compact operators A = I + K and $A_0 = I - K$ by employing a collocation method. The collocation method restricts our solution space for (6) to a finite dimensional space and enforces equality at a finite set of collocation points. To this end, let $\{\phi_i\}_{i=1}^N$ be a set of linearly independent functions corresponding to a discretization of our rescaled scattering obstacle \bar{S} into the volumes $\{d_i\}_{i=1}^N$, where the points $\{\mathbf{s}_i\}_{i=1}^N = \{(\mathbf{x}, \xi)_i\}_{i=1}^N$ are midpoints of the discretization volumes.

For the sake of presenting this idea in the simplest way, we use piecewise constant basis functions ϕ_j ($\phi_j(x) = 1$ if $x \in d_j$, and zero otherwise) and solve for $\tilde{u} \in$ span $\{\phi_i\}_{i=1}^N$ by requiring equality at the collocation points \mathbf{s}_i for $i = 1, \ldots, N$. This gives the linear system

$$(\mathbf{I} - \mathbf{K})\mathbf{u} = \mathbf{u}^i$$

where

$$\begin{split} \mathbf{K}_{ij} &= \kappa^2 \int_{d_j} (h - \epsilon(\mathbf{s}')) \overline{G}(\mathbf{s}_i, \mathbf{s}') \, d\mathbf{s}', \\ \mathbf{u}_i^i &= \overline{u}^i(\mathbf{s}_i). \end{split}$$

We evaluate each entry \mathbf{K}_{ij} using a Clenshaw–Curtis quadrature scheme [4].

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4.1. Solving the preconditioned system. Applying the same collocation method to the preconditioner operator $A_0 = I - K_0$, we get a preconditioning matrix

$$\mathbf{I}-\mathbf{K}_{0},$$

where

$$(\mathbf{K}_0)_{ij} = \kappa^2 \int_{d_j} \epsilon(\mathbf{s}') G_0(\mathbf{s}_i, \mathbf{s}') \, d\mathbf{s}'.$$

Note that the integral defining $(\mathbf{K}_0)_{ij}$ integrates over the Ω and z direction, but the integrand is constant in the z direction. Therefore the matrix will have the tiled structure

(12)
$$\mathbf{K}_{0} = d_{z} \begin{bmatrix} \mathbf{K}_{2D} & \mathbf{K}_{2D} & \cdots & \mathbf{K}_{2D} \\ \vdots & \ddots & & \\ \vdots & & \ddots & \\ \mathbf{K}_{2D} & \mathbf{K}_{2D} & \cdots & \mathbf{K}_{2D} \end{bmatrix},$$

where \mathbf{K}_{2D} corresponds to the discretization of the integral operator

$$(K_{2D}u)(\mathbf{x}) = \kappa^2 \int_{\Omega} \epsilon_0(\mathbf{x}') G_0(\mathbf{x}, \mathbf{x}') u(\mathbf{x}') \, d\mathbf{x}',$$

 $d_z = 1/m$ is the height of the discretization volumes, and m is the number of discretizations in the z direction. Thus

$$(\mathbf{K}_{2D})_{ij} = \kappa^2 \int_{\omega_j} \epsilon_0(\mathbf{x}') G((\mathbf{x}_i, 0), (\mathbf{x}', 0)) \, d\mathbf{x}',$$

where $\{\omega_j\}_{j=1}^n$ is a discretization of Ω corresponding to the discretization of $\Omega \times [-1/2, 1/2]$ into $\{d_j\}_{j=1}^n$. The entries of \mathbf{K}_{2D} are approximated using Clenshaw–Curtis quadrature.

4.2. Solving the discretized preconditioner as a two dimensional problem. The linear algebra analogue to the method we used to pose the preconditioning operator as a two dimensional problem derives from taking advantage of the tiling effect of \mathbf{K}_0 The preconditioning step involves solving, for arbitrary data \mathbf{z} ,

$$\mathbf{y}_k - \frac{1}{m} \mathbf{K}_{2D} \sum_{i=1}^m \mathbf{y}_i = \mathbf{z}_k$$
 for $k = 1, \dots, m$,

where m is the number of discretizations in the z direction. Note that for our regular discretization, $d_z = 1/m$. In section 2.1 we show that the preconditioning step can be solved as a two dimensional system by a continuous average in the z direction. The analogue to that approach for the discretized system of equations can be expressed by

$$\frac{1}{m}\sum_{k=1}^{m}\mathbf{y}_{k} - \frac{1}{m}\mathbf{K}_{2D}\sum_{i=1}^{m}\mathbf{y}_{i} = \frac{1}{m}\sum_{k=1}^{m}\mathbf{z}_{k}.$$

Let

$$\mathbf{y}_a = \frac{1}{m} \sum_{k=1}^m \mathbf{y}_k,$$
$$\mathbf{z}_a = \frac{1}{m} \sum_{k=1}^m \mathbf{z}_k.$$

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B1016



FIG. 3. For $\kappa = 2$, $\varepsilon_0 = 1$ and $h = 10^{-1}$, 10^{-2} , 10^{-3} , and 10^{-4} , left to right and top to bottom, we plot the relative residuals in the solid black line and, if applicable, the bound $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2^m$ in a dashed line.

This gives the matrix equation on the order of the individual blocks

$$(\mathbf{I} - \mathbf{K}_{2D})\mathbf{y}_a = \mathbf{z}_a.$$

We reconstruct each \mathbf{y}_k from the solution to this system by

$$\mathbf{y}_k = \mathbf{z}_k + \mathbf{K}_{2D} \mathbf{u}_a$$

= $\mathbf{z}_k - \mathbf{z}_a + \mathbf{y}_a$.

This implies that $\mathbf{A}_0^{-1} = (1/m)\mathbf{E} \otimes (\mathbf{A}_{2D}^{-1} - \mathbf{I}) + \mathbf{I}$, where $\mathbf{A}_{2D} = \mathbf{I} - \mathbf{K}_{2D}$ and \mathbf{E} is the $m \times m$ matrix of all ones and \otimes is the Kronecker product.

5. Numerical results. To demonstrate the effectiveness of the preconditioning scheme presented in the previous section, we present the results of several numerical experiments in this section. For all problems in the section, the scattering obstacle is a square slab that is $\kappa \times \kappa$ wavelengths with width h. That is, the scattering obstacle $S = \Omega \times [-h/2, h/2]$, where Ω is the $2\pi \times 2\pi$ square. The grid used for discretization is $40 \times 40 \times 7$.

The number of Chebyshev nodes used to compute each matrix entry is 3^2 for the two dimensional grid and 3^3 for the three dimensional grid. The refractive index is constant. Figure 3 illustrates the relative residual norm for the first ten iterates of the GMRES method, as well as the bound for the residual $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2^m$ at each iteration m if applicable.



FIG. 4. GMRES iteration counts as a function of h for k = 2, 4, 6, 8 (left to right, top to bottom). The solid black line gives the iteration count for the preconditioned system. The solid grey line gives the iteration count for the unpreconditioned system. The maximum iteration was set to 600. The dashed line gives the iteration bound $\lceil \log_{\varepsilon}(10^{-8}) \rceil$ if the bound is less than 600 and $\varepsilon := ||\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}||_2 < 1$. For this problem $\varepsilon_0 = 1$ and the right-hand side vector was randomly generated by the randn function in MATLAB.

GMRES shows considerable improved performance when applied to the preconditioned system compared to the original discretized system for sufficiently thin inhomogeneities. Figures 4 and 5 show that for values of $h < 10^{-1}$ (and sometimes for thicker inhomogeneities), we begin to get a substantial reduction in the number of GMRES iterations required for convergence. Furthermore, the numerical experiments show that the bounds demonstrated in Corollary 4 are effective at predicting the fast convergence for the preconditioned problem. The corollary suggests that the number of iterations required for convergence can be bounded by $\lceil \log_{\varepsilon}(tol) \rceil$ if $\varepsilon := \|\mathbf{I} - \mathbf{A} \mathbf{A}_0^{-1}\|_2 < 1$. In all the numerical experiments presented here, the tolerance for the relative residual is set to $tol = 10^{-8}$.

Figure 5 illustrates the iterations necessary for convergence for the preconditioned and unpreconditioned system as well as the iteration bound we've developed. For this experiment, the refractive index is nonconstant and periodic and is given by

$$\varepsilon_0(\mathbf{x}) = 1 + |\sin(3x_1)\sin(3x_2)|.$$

6. Conclusion and further work. Building thin, photonic band gap media with a two dimensional periodic structure is important to power and material reduction [19]. Therefore the efficient computational modeling of time harmonic scattering through such media is useful to such applications as the field of optics. We have shown



FIG. 5. GMRES iteration counts as a function of h for k = 2, 3, 4, 5 (left to right, top to bottom). The solid black line gives the iteration count for the preconditioned system. The solid grey line gives the iteration count for the unpreconditioned system. The maximum iteration was set to 600. The dashed line gives the iteration bound $\lceil \log_{\varepsilon}(10^{-8}) \rceil$ if the bound is less than 600 and $\varepsilon := ||\mathbf{I} - \mathbf{AA}_0^{-1}||_2 < 1$. For this problem $\varepsilon_0(x_1, x_2) = 1 + |\sin(3x_1)\sin(3x_2)|$.

that the asymptotic results in [13] can be used effectively to develop preconditioning systems for solving the full three dimensional scattering problem for waveguides with lengths less than 10^{-1} in the thin direction (and sometimes larger). Implementing such a preconditioner however required a novel implementation that allows inner solves to be carried out in two dimensional complexity yet still resolve three dimensional data. We have also developed asymptotic spectral bounds and GMRES bounds that give some indication when this preconditioning method will be effective.

This problem is rich in opportunities for further work. The thin geometry of the inhomogeneity and the typical periodic structure of the refractive index suggest that there are meshes that would perform better than the regular meshes used in the numerical examples presented here. Furthermore, high resolution meshes would require developing fast integral methods for this iterative approach to be feasible. An efficient and fast integral algorithm would allow one to compute the matrix vector products required at each step of the GMRES process at less than $O(N^2)$ complexity (see, e.g., [1, 3, 8, 7, 14, 15]). The examples included in this paper are low resolution and are included to illustrate the bounds we have derived. To suit this problem, such an approach would have to align an efficient mesh configuration with the tiled format demonstrated in (12). It is important to point out, however, that if one were to employ a Nyström discretization (rather than a collocation method like one used here), one would have to take care of vertically aligned, but unequal, vertices of the mesh, since as $h \rightarrow 0$, the Green's function approaches a singularity that wouldn't appear in the two dimensional discretization, implying that our preconditioner no longer approximates an inverse. However, we are confident that one can significantly accelerate the integral computations with a high order of accuracy and utilize the preconditioning method described here to produce a high order and efficient method for solving this problem. Such a result would be a significant and welcome contribution.

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