A PRECONDITIONING METHOD FOR THIN HIGH CONTRAST SCATTERING STRUCTURES

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We present a method to precondition the discretized Lippmann-Schwinger integral equations which model time-harmonic scalar waves in the presence of a thin inhomogeneous scatterer of high contrast. The preconditioner is based on asymptotic results as the thickness of the third component direction goes to zero and requires solving a two dimensional limiting formulation of the problem at the preconditioning step.

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

AMS subject classifications. 65F08, 65F10, 15A018, 47A10, 47A55

1. Introduction.

We consider the problem of scattering of time-harmonic scalar waves through a thin structure of high contrast in three dimensions. Such a model arises in the study of photonic band gap structures. Photonic band gap materials are designed to guide the propagation of light by blocking certain wavelengths (the band gap), while allowing others to pass freely through, facilitating information propagation in optical communication networks and in optical computing. We consider here three dimensional slab waveguides with a two dimensional photonic crystal structure. Slab materials are typically constructed with a high refraction index and are embedded in a homogenous scattering medium, typically air. See [22], [23], [9] for more on thin photonic band gap structures.

We assume here that the wave phenomenon is modeled by the Helmholtz equation, keeping in mind that the full Maxwell equations are needed for three dimensional photonics. We solve the Helmholtz equation by discretizing its equivalent Lippmann-Schwinger volume integral equation formulation [8]. The resulting finite dimensional linear system is large, dense, and non-Hermitian. While there are efficient matrix-vector product routines that make an iterative solver an appealing approach [4, 6, 11, 10, 17, 18], spectral properties of the system often cause Krylov subspace based iterative methods to converge slowly.

In [16] the authors proposed an asymptotic expansion of the Lippmann-Schwinger integral equation for inhomogeneities that are simultaneously high contrast and thin in one component direction. They showed that the the solution to a two dimensional effective model 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. We 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 describe how to do this in section 2. We then apply the asymptotic results from [16] to obtain bounds on the GMRES residual applied to

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the preconditioned system in section 3. We discuss the numerical implemention in section 4, and finally in section 5, we demonstrate its effectiveness with numerical examples.

1.1. Problem Formulation. We consider a (potentially inhomogeneous) scatterer $S \in \mathbb{R}^3$, thin in the third component direction, and set in a homogenous host medium such as air or some fluid. The total scattered field u is satisfies the Helmholtz equation

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

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 condtion, which implies there is no wave reflection at infinity [8]:

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

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

We are most interested in two dimensionally periodic photonic crystal structures in a three dimensional scattering thin slab, so the refractive index is assumed to be constant in the thin component direction. As in [16], we assume the scatterer is of the form

$$S = \Omega \times [-h/2, h/2]$$

and let $s = (\mathbf{x}, z)$ for $\mathbf{x} \in \Omega$, Ω a bounded domain in $\mathbb{R}^2$ and $z \in [-h/2, h/2]$. We model the high contrast of the squared refractive index as $\epsilon_0(\mathbf{x})/h$, where h is the length of the thin side, an appropriate regime for thin slab photonic band gap structures, where $\epsilon_0(\mathbf{x})$ models the inhomogeneous two dimensionally periodic structure. Thus we define the squared refractive index function

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

so that $\epsilon - 1$ is compactly supported on the scatterer S. If $u = u^s + u^i$ satisfies equations (1) and (2), then u is also a solution to the Lippmann-Schwinger volume integral equation [8]

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

where $G(\mathbf{s})$ is the free space Green's function given by

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

Using that the scatterer $S = \Omega \times [-h/2, h/2]$ 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

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

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

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

where

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

We define our rescaled domain $\tilde{S} = \Omega \times [-1/2, 1/2]$, and note that the above $K : L^\infty(\tilde{S}) \to L^\infty(\tilde{S})$ is compact.

2. Application of the GMRES iterative method. Consider applying the GMRES iterative method [19] to the continuous equation (6). Since the operator we are interested in is of the form $A := I + K$, where K is compact, A is bounded and has only a finite spectrum outside any neighborhood of one [14, pg. 421]. Thus, unlike discretizations of the Helmholtz equation (1), refining the discretizations of the Lippmann-Schwinger equation has little effect on the conditioning of the resulting linear system and therefore little effect on GMRES performance [13], [12]. Numerical experiments in [20] show that increased mesh resolution only adds high frequency eigenmodes to the spectrum, corresponding to eigenvalues of A close to one. Thus we should expect that convergence analysis of the continuous case gives insight to convergence behavior of the discretized problem, see e.g. [5, 15, 21, 24].

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

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

where $\mathcal{K}_m(A, u^i) := \text{span}\{u^i, Au^i, A^2u^i, \cdots, A^{m-1}u^i\}$ is the Krylov subspace and $\|\cdot\|$ is an appropriate operator norm. In our paper, and following the results in [16], we will use the $L^\infty(X)$ vector norm and the operator norm it induces, where is 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 the minimizer u_m as a product of a polynomial evaluated at A of degree $m - 1$ and the incident wave u^i. 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, and the polynomial is equal to 1 at the origin. Then equation 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 which are equal to 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 [19], therefore the cost per iteration and memory requirements grows with each iteration as one must store the basis for the growing Krylov subspace. Thus GMRES is feasible if the number of iterations remain small, but may be too computationally expensive without effective preconditioning.

Now we apply the asymptotic results of [16] to build an effective preconditioning scheme. That is, rather than apply GMRES to equation (6), we solve the equivalent problem

$$\left(AA_0^{-1}\right)(A_0 u) = u^i,$$

where a substantially lower order polynomial in $\mathcal{P}_m^0$ is necessary to achieve small residual when evaluated at AA_0^{-1}, and one can solve $A_0 y = z$ relatively quickly for an arbitrary function $z \in C(\tilde{S})$ (here A_0 will be from a two dimensional problem). In this case, the right hand side data need not have physical meaning; in fact it is 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

$$(I - K_{2D})u_0(\mathbf{x}) = u^i(\mathbf{x},0) \tag{8}$$

where

$$(K_{2D}u_0)(\mathbf{x}) := \kappa^2 \int_\Omega \epsilon_o(\mathbf{x}')G((\mathbf{x},0),(\mathbf{x}',0))u_0(\mathbf{x}')\,d\mathbf{x}'. \tag{9}$$

This is the negative of the two dimensional limiting operator for (7). Note, however, that in order to use (8) as a preconditioner, we must extend its domain to include functions on $\tilde{S} = \Omega \times [-1/2, 1/2]$. Thus we define $K_0 : C(\tilde{S}) \to C(\tilde{S})$ by

$$(K_0 u)(\mathbf{x},\eta) = K_{2D}\left(\int_{-1/2}^{1/2} u(\mathbf{x},\eta)\,d\eta\right) \tag{10}$$

Note that the domain of K_0 contains continuous functions on the the three dimensional compact set $\tilde{S}$, but its image contains only functions that are constant in the z direction. Then the preconditioning operator is defined to be $A_0 := I - K_0$. Lemma 2 of [16] shows that A_0 is continuously invertible on both $L^2(\tilde{S})$ and $C(\tilde{S})$.

2.1. The preconditioning step. 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 $(A_0 y)(s) = z(s)$, 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, which of course will have much lower computational cost than the original three dimensional problem.

This issue is quite easily dealt with; note that if $(A_0 y)(s) = z(s)$, 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 its z average $\int_{-1/2}^{1/2} y(\mathbf{x},\zeta) - z(\mathbf{x},\zeta)\,d\zeta$. This gives us the equation

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

which can be rearranged to be

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

Define

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

and

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

Then the preconditioning step is equivalent to solving the two dimension 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 obtain our desired solution by setting

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

That is, the z direction variations in the right hand side are simply added back into the two dimensional solutions.

3. Asymptotic Results.

We present here the main result from [16] and extend it to obtain GMRES convergence bounds when applied to equations (8) and (9).

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

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

Proof. See [16, Lemma 1]

It's follows from Lemma 1 of [16], 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 $M \le \pi d$, where $d = \mathrm{diam}(\Omega)$. 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 (10). There exists a constant C', independent of h, but depending on κ such that*

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

Proof.

$$\begin{aligned} \|I - AA_0^{-1}\| &= \|(A_0 - A)A_0^{-1}\| \\ &\le \|A_0^{-1}\|\|A_0 - A\| \end{aligned}$$

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

$$\begin{aligned}\|A - A_0\| &= \sup_{\|u\|=1} \|A_0 u - Au\| \\ &= \sup_{\|u\|=1} \|K_0 u + Ku\|\end{aligned}$$

which can be bounded to obtain

$$\begin{aligned}(11)\quad \|A - A_0\| \le \sup_{\|u\|=1} \sup_{(\mathbf{x},\zeta)\in\tilde{S}} \Bigg(& h\kappa^2 \int_{-1/2}^{1/2} \int_\Omega |G((\mathbf{x},0),(\mathbf{x}',0))|\,|u(s')|\,ds' \\ & + h\kappa^2 \int_{-1/2}^{1/2} \int_\Omega |G((\mathbf{x},0),(\mathbf{x}',0)) - G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))|\,|u(\mathbf{x}',\zeta')|\,d\zeta' d\mathbf{x}' \\ & + \kappa^2 \int_{-1/2}^{1/2} \int_\Omega \epsilon_0(\mathbf{x}')\,|G((\mathbf{x},0),(\mathbf{x}',0)) - G((\mathbf{x},h\zeta),(\mathbf{x}',h\zeta'))|\,|u(\mathbf{x}',\zeta')|\,d\zeta' d\mathbf{x}' \Bigg) \\ & \le h\kappa^2 \left(\frac{M}{4\pi} + Ch + C\|\epsilon_0\|_{L^\infty(\Omega)} \right).\end{aligned}$$

Therefore, $\|I - AA_0^{-1}\|$ is small if the scattering medium is sufficiently thin. Note that this bound depends on the constant $\|A_0^{-1}\|$, which, while independent of h, could possibly be very large. However, in practice we see that $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|$ is much smaller than the bounds above, where $\mathbf{A}$, and $\mathbf{A}_0$ are discretizations of A and A_0 respectively. The discretized operators are obtained by using a collocation method, which we describe in section 4. We plot the computed values of $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|$ in Figure 1.

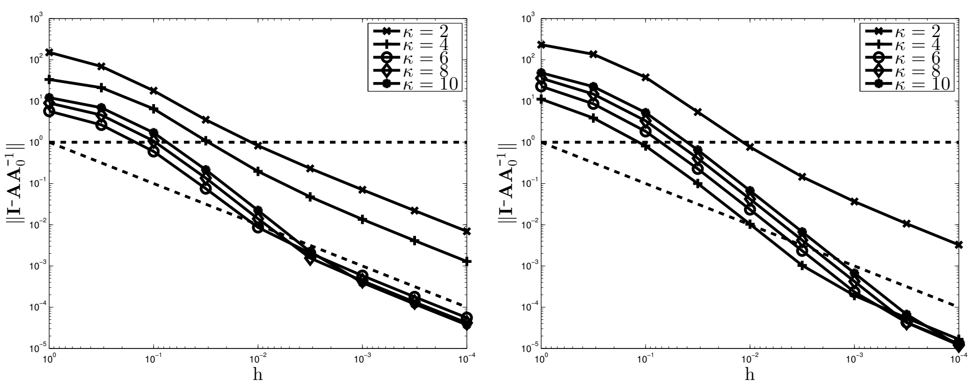

FIG. 1. $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|$ *for* $\epsilon_0 = 3$ *on left,* $\epsilon_0 = 9$ *on right.*

The reason the results are better than the above estimate is that by factoring out the inverse of the preconditioning operator A_0, we didn't take into account spectral deflating. 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. The numerical results in Figure 1 suggest that we not only approximate well the eigenvalues, but also those 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 demonstrate that $\sigma(\mathbf{A}\mathbf{A}_0^{-1}) \to 1$ 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 (10), 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

$$\begin{aligned}
\|(\lambda - A)v_0\|_{L^\infty(\tilde{S})} = &\Bigg| \sup_{(\mathbf{x},\zeta)\in\tilde{S}} \kappa^2 h \int_{\tilde{S}} G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta'))v_0(\mathbf{x}')\, d\zeta' d\mathbf{x}' \\
&+\kappa^2 \int_\Omega \int_{-1/2}^{1/2} \epsilon_0(\mathbf{x}')\left(G((\mathbf{x}, 0), (\mathbf{x}', 0)) - G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta'))\right) v_0(\mathbf{x}')\, d\zeta' d\mathbf{x}' \Bigg| \\
\leq &\, h \sup_{(\mathbf{x},\zeta)\in\tilde{S}} \left| \kappa^2 \int_{\tilde{S}} G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta'))v_0(\mathbf{x}')\, d\zeta' d\mathbf{x}' \right| \\
&+ \sup_{(\mathbf{x},\zeta)\in\tilde{S}} \kappa^2 \int_\Omega |\epsilon_0(\mathbf{x}')|\, |v_0(\mathbf{x}')| \int_{-/12}^{1/2} |G((\mathbf{x}, 0), (\mathbf{x}', 0)) - G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta'))|\, d\zeta' d\mathbf{x}' \\
\leq &\, h\|K(\epsilon_0 = 1)\|_{L^\infty(\tilde{S})} + Ch\|\epsilon_0\|_{L^\infty(\Omega)},
\end{aligned}$$

where C is the constant from theorem 1.

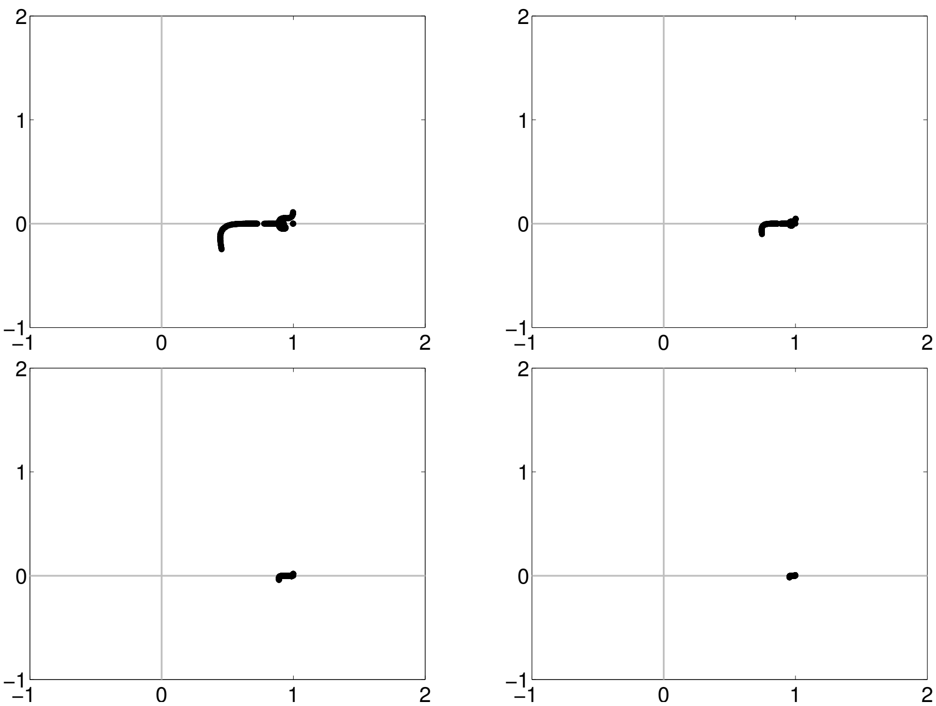

FIG. 2. *The spectrum $\sigma(\mathbf{A}\mathbf{A}_0^{-1})$ for values of $h = 10^{-1}, 10^{-1.2}, 10^{-1.4}, 10^{-1.6}$ going left to right, top to bottom.*

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 (10). Then the relative residual of the GMRES* *problem applied to the right preconditioned problem*

$$\left(AA_0^{-1}\right)(A_0 u) = u^i,$$

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

Proof. Recall that we can bound the GMRES residual by the minimum of all polynomials in $\mathcal{P}_m^0$ evaluated at AA_0^{-1},

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

In particular we can take $p_m(x) = (1-x)^m$, and use Corollary 2 to obtain

$$\begin{aligned}\frac{\|r_m\|}{\|u^i\|} &\leq \|(I - AA_0^{-1})^m\| \\ &\leq \|I - AA_0^{-1}\|^m \\ &\leq \epsilon^m\end{aligned}$$

where $\epsilon = O(h)$.

4. Numerical Implementation. Recall that we denote the rescaled slab by $\tilde{S} := \Omega \times [-1/2, 1/2]$. For a function f defined on $S = \Omega \times [-h/2, h/2]$ on S, we denote by $\tilde{f} : \tilde{S} \to \mathbb{C}$ the scaled function $\tilde{f}(\mathbf{s}) := \tilde{f}((\mathbf{x}, \zeta)) := f((\mathbf{x}, h\zeta))$ for $\mathbf{s} \equiv (\mathbf{x}, \zeta) \in \tilde{S}$. That is,

$$\begin{aligned}\tilde{G}(\mathbf{s}, \mathbf{s}') &:= \tilde{G}((\mathbf{x}, \zeta), (\mathbf{x}, \zeta)') := G((\mathbf{x}, h\zeta), (\mathbf{x}, h\zeta)'), \\ \tilde{u}^i(\mathbf{s}) &:= \tilde{u}^i((\mathbf{x}, \zeta)) := u^i((\mathbf{x}, h\zeta)).\end{aligned}$$

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

$$\begin{aligned}G_0(\mathbf{s}, \mathbf{s}') &:= G((\mathbf{x}, 0), (\mathbf{x}', 0)) \\ u_0^i(\mathbf{s}) &:= u^i((\mathbf{x}, 0)).\end{aligned}$$

We discretize our shifted compact operators $A = I + K$, and $A_0 = I - K_0$ using a collocation method. That is, we restrict our solution space for (6) to a finite dimensional subspace, and enforce equality at a finite set of collocation points. To this end, let $\{\phi_i\}_{i=1}^N$ be a set of linear 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.

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

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

where

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

We evaluate each entry $\mathbf{K}_{ij}$ using a Clenshaw-Curtis quadrature scheme [7].

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, however the integrand is constant in the z direction. Therefore the matrix will have the tiled structure

$$\mathbf{K}_0 = d_z \begin{bmatrix} \mathbf{K}_{2D} & \mathbf{K}_{2D} & \cdots & \mathbf{K}_{2D} \\ \vdots & \ddots & & \\ \vdots & & \ddots & \\ \mathbf{K}_{2D} & \mathbf{K}_{2D} & \cdots & \mathbf{K}_{2D} \end{bmatrix}, \tag{12}$$

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

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

and d_z is the height of the discretization volumes. 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.

As an analog to the continuous case, we take advantage of the tiled structure of $\mathbf{K}_0$ to reduce the complexity. The preconditioning step involves solving, for arbitrary data $\mathbf{z}$

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

where m is the number of discretizations in the z direction. Note that for our regular discretization, $d_z = 1/m$. Then, as a discrete analog of averaging in the z direction, we rewrite the above set of matrix equations to get

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

Let

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

and

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

This yields the matrix equation on the individual blocks

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

from which we then reconstruct each $\mathbf{y}_k$ from the solution to this system by

$$\begin{aligned}\mathbf{y}_k &= \mathbf{z}_k + \mathbf{K}_{2D}\mathbf{u}_a \\ &= \mathbf{z}_k - \mathbf{z}_a + \mathbf{y}_a\end{aligned}$$

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

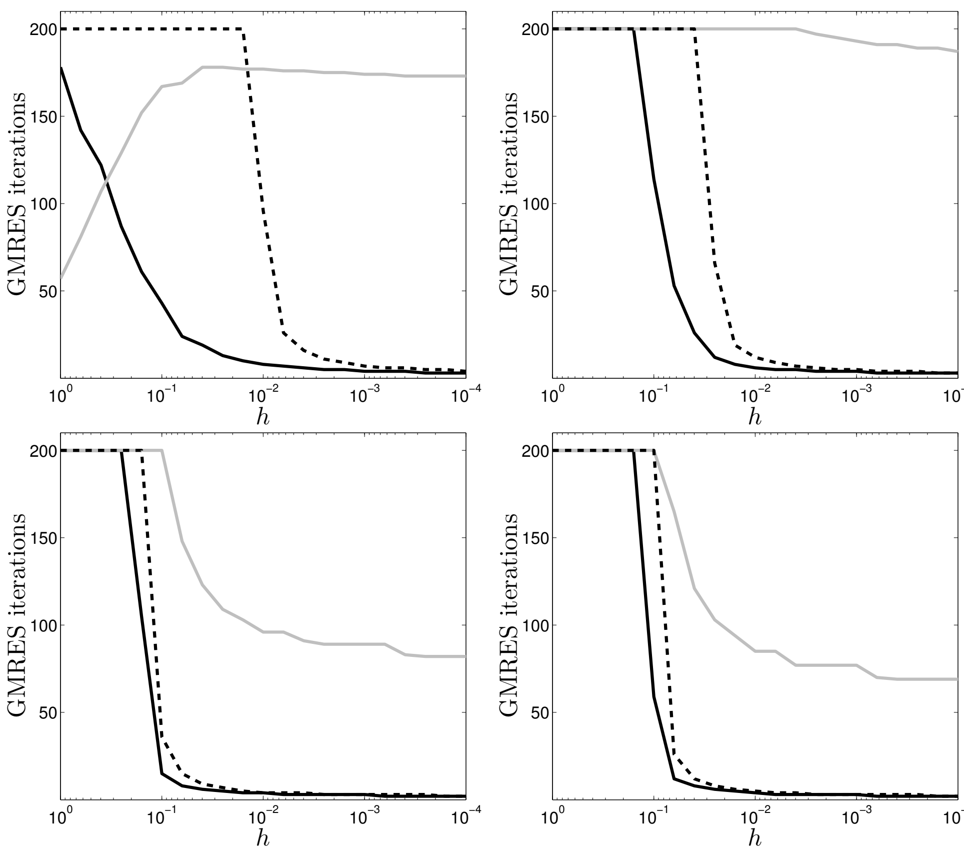

FIG. 3. *GMRES Iteration counts as a function of h for $k = 2, 4, 6, 8$ (left to right, top to bottom). The solid black line gives the iteration count for the preconditioned system. The solid grey line gives the iteration count for the unpreconditioned system. The maximum iteration was set to 200. The dashed line gives the iteration bound $\lceil \log_\varepsilon(10^{-8}) \rceil$ if the bound is less than 200 and $\varepsilon := \|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2 < 1$. For this problem $\varepsilon_0 = 3$ and the right hand side vector was randomly generated by Matlabs* `randn` *function.*

5. Numerical Results. To demonstrate the effectiveness of the preconditioning scheme presented in the previous section, here we present the results of several numerical experiments. For all of the examples in this section, the scattering obstacle is a square cylinder with height h, and the grid used for discretization is $24 \times 24 \times 7$.

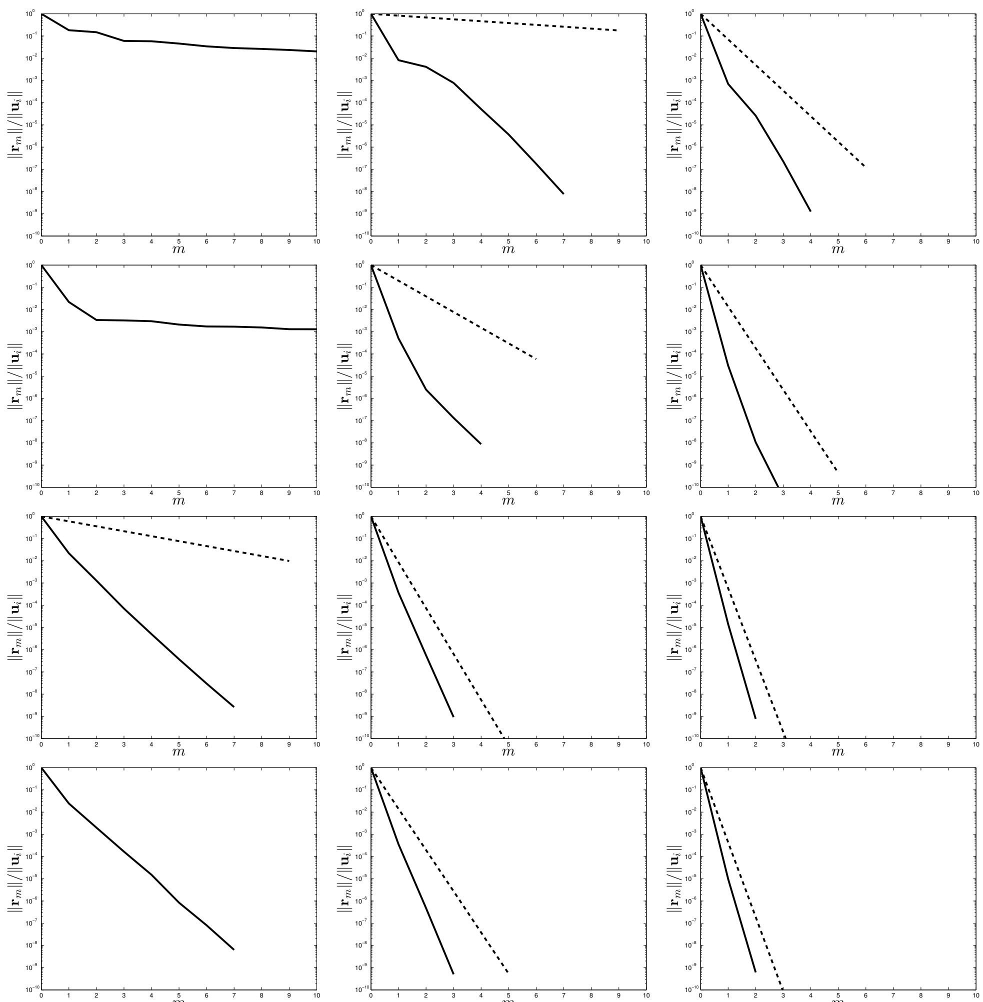

FIG. 4. *For $\kappa = 2, 4, 6, 8$ top to bottom and $h = 10^{-1}, 10^{-2}, 10^{-3}$ left to right, we plot the first 10 relative residuals and in the solid black line and, if applicable, the bound $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2^m$ in a dashed line. For this problem $\epsilon_0 = 3$ and the right hand side vector is a discretization of a plane wave of wave number κ traveling in the x direction.*

GMRES shows considerable improved performance when applied to the preconditioned system compared to the original discretized system for sufficiently thin inhomogeneities. Figures 3 and 5 show that for values of h near 10^{-1} (and sometimes for thicker inhomogeneities), we begin to get 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 $tol = 10^{-8}$.

For the first set of experiments, 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, and the refractive index is constant within the scatterer. Figure 4 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.

For our next example, the refractive index is periodic and is given by

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

The number of Chebyshev nodes used to compute each matrix entry is 5^2 for the two dimensional grid and 5^3 for the three dimensional grid. Figure 5 illustrates the iterations necessary for convergence for the preconditioned and unpreconditioned system as well as the predicted iteration bound.

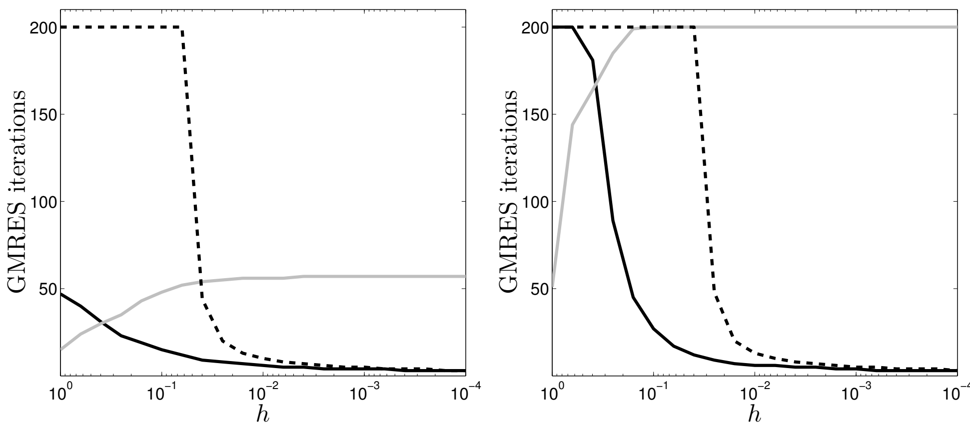

FIG. 5. *GMRES Iteration counts as a function of h for k = 2, 4, 6, 8 (left to right, top to bottom). The solid black line gives the iteration count for the preconditioned system. The solid grey line gives the iteration count for the unpreconditioned system. The maximum iteration was set to 200. The dashed line gives the iteration bound $\lceil \log_\varepsilon(10^{-8})\rceil$ if the bound is less than 200 and $\varepsilon := \|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2 < 1$. For this problem $\varepsilon_0(x, y) = 1 + |\sin(x)\sin(y)|$ and the right hand side vector is a discretization of a plane wave of wave number κ traveling in the x direction.*

6. Conclusion and Further Work.

Analyzing thin, photonic band gap media with two dimensional periodic structures is important for novel optical material design [22], and the efficient computational modeling of wave propagation through such media will be important to render three dimensional computations feasible. We have shown that the asymptotic results in [16] can be used effectively to precondition the full three dimensional scattering problem for waveguides with small thickness. Such a preconditioner allows inner solves to be carried out in two dimensional complexity for a three dimensional problem. We have also developed asymptotic spectral bounds and GMRES bounds that give some indication when this preconditioning method will be effective.

Similar limiting formula for thin high contrast scatterers have been obtained for Maxwell equations [3], [2],[1], and the implementation of the analogous preconditioner to fully resolve electromagnetic waves in three dimensions is the subject for future work. Furthermore, thin geometry and high contrast of the inhomogeneity suggest the use of more efficient meshes than the regular meshes used in the numerical examples presented here. High resolution meshes will require the implementation fast integral methods for this iterative approach to be feasible. An efficient and fast integral algortihm would allow one to compute the matrix vector products required at each step of the GMRES process at less than $\mathcal{O}(N^2)$ complexity (see e.g. [4, 6, 11, 10, 17, 18]). The examples included in this paper are low resolution and are included to illustrate the effectiveness of the preconditioner and the sharpness of the bounds.

REFERENCES

[1] D. M. Ambrose, J. Gopalakrishnan, S. Moskow, and S. Rome, *Scattering of electromagnetic waves by thin high contrast dielectrics ii: asymptotics of the electric field and a method for inversion.* to appear *Comm. Math. Sci.*

[2] D. M. Ambrose and S. Moskow, *Scattering of electromagnetic waves by thin high contrast dielectrics: effects of the object boundary*, Commun. Math. Sci., 11 (2013), pp. 293–314.

[3] H. Ammari, H. Kang, and F. Santosa, *Scattering of electromagnetic waves by thin dielectric planar structures.*, SIAM J. Math. Anal., 38 (2006), pp. 1329–1342.

[4] O. Bruno and A. Sei, *A fast high-order solver for em scattering from complex penetrable bodies: Te case*, Antennas and Propagation, IEEE Transactions on, 48 (2000), pp. 1862–1864.

[5] Z.-H. Cao, *A note on the convergence behavior of GMRES*, Appl. Num. Math., 25 (1997), pp. 13–20.

[6] Y. Chen, *A fast, direct algorithm for the lippmann-schwinger integral equation in two dimensions.*, Advances in Computational Mathematics, 16 (2002), pp. 175–190.

[7] C. W. Clenshaw and A. R. Curtis, *A method for numerical integration on an automatic computer*, Numer. Math., 2 (1960), pp. 197–205.

[8] D. Colton and R. Kress, *Inverse Acoustic and Electromagnetic Scattering Theory*, Springer-Verlag, Berlin, 1998.

[9] S. Fan, J. Winn, A. Devenyi, J. Chen, R. Meade, and J. Joannopoulos, *Guided and defect modes in periodic waveguides*, J. Opt. Soc. Amer. B Opt. PHys., 12 (1995), pp. 1267–1283.

[10] L. Greengard and V. Rokhlin, *A fast algorithm for particle simulations*, Journal of Computational Physics, 135 (1997), pp. 280 – 292.

[11] E. M. Hyde and O. P. Bruno, *An efficient, preconditioned, high-order solver for scattering by two-dimensional inhomogeneous media*, J. Comp. Phys., 200 (2004), pp. 670–694.

[12] ———, *A fast, higher-order solver for scattering by penetrable bodies in three dimensions*, J. Comp. Phys., 202 (2005), pp. 236–261.

[13] C. Johnson, *Numerical Solution of Partial Differential Equations by the Finite Element Method*, Cambridge University Press, Sweden, 1995.

[14] E. Kreyszig, *Introductory Functional Analysis with Applications*, Wiley, New York, 1989.

[15] I. Moret, *A note on the superlinear convergence of GMRES*, SIAM J. Num. Anal., 34 (1997), pp. 513–516.

[16] S. Moskow, F. Santosa, and J. Zhang, *An approximate method for scattering by thin structures*, SIAM J. Appl Math., 66 (2005), pp. 187–205.

[17] K. Nabors, F. T. Korsmeyer, F. T. Leighton, and J. White, *Preconditioned, adaptive, multipole-accelerated iterative methods for three-dimensional first-kind integral equations of potential theory*, SIAM J. Sci. Comput., 15 (1994), pp. 713–735.

[18] V. Rokhlin, *Rapid solution of integral equations of scattering theory in two dimensions*, Journal of Computational Physics, 86 (1990), pp. 414 – 439.

[19] Y. Saad and M. H. Schultz, *GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM J. Sci. Stat. Comp., 7 (1986), pp. 856–869.

[20] J. Sifuentes, *Preconditioning the integral formulation of the helmholtz equation via deflation*, Master's thesis, Rice University, 2006.

[21] V. Simoncini and D. B. Szyld, *On the occurrence of superlinear convergence of exact and inexact Krylov subspace methods*, SIAM Review, 47 (2005), pp. 247–272.

[22] P. Villeneuve, S. Fan, S. Johnson, and J. Joannopoulos, *Three-dimensional photon confinement in photonic crystals of low-dimensional periodicity*, IEE Proc. Optoelectron, 145 (1998), pp. 384–390.

[23] J. Vuckovic, M. Loncar, H. Mabuchi, and A. Scherer, *Optimization of the q factor in photonic crystal microwavities*, IEEE J. Quantum Elec., 38 (2002), pp. 850–856.

[24] R. Winther, *Some superlinear convergence results for the conjugate gradient method*, SIAM J. Num. Anal., 17 (1980), pp. 14–17.