

# PRECONDITIONING METHODS FOR THIN SCATTERING STRUCTURES BASED ON ASYMPTOTIC RESULTS

JOSEF A. SIFUENTES<sup>§</sup> AND SHARI MOSKOW<sup>†</sup>

10 February 2018

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

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

11 **1. Introduction.** We consider the problem of scattering time-harmonic acoustic  
 12 waves through thin, three dimensional inhomogeneities. This physical phenomenon is  
 13 relevant in the study of photonic band gap structures. Such structures are designed to  
 14 guide the propagation of light by blocking certain wavelengths in the band gap, while  
 15 allowing others to pass freely through. Such structures facilitate information propagation  
 16 in optical communication networks and in optical computing. We consider three  
 17 dimensional slab waveguides with two dimensional photonic crystal structure. Such  
 18 structures are typically constructed with a high refraction index and are imbedded in  
 19 a homogenous scattering medium, typically air. See [19], [20], [6] for more on thin  
 20 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, however there are efficient matrix-vector 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  $h \rightarrow 0$ , 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 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 implementation 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

<sup>†</sup>Department of Mathematics, Drexel University, Korman Center 33rd and Market St., Philadelphia, PA 19104 ([moskow@math.drexel.edu](mailto:moskow@math.drexel.edu)).

<sup>§</sup>School of Mathematical and Statistical Sciences, University of Texas - Rio Grande Valley, 1201 West University Dr, Edinburg, TX 78539-2999 ([josef.sifuentes@utrgv.edu](mailto:josef.sifuentes@utrgv.edu)).

41 effectiveness of the preconditioner to significantly improve convergence speed and the  
 42 efficacy of the bounds we develop.

43 **1.1. Problem Formulation.** We consider the setting of an inhomogenous scat-  
 44 tering medium  $S \in \mathbb{R}^3$ , thin in the third component direction, and set in a homogenous  
 45 host medium such as air or some fluid. Let  $S$  be the cartesian cross product of its two  
 46 dimensional cross section,  $\Omega$  and the thin, third component direction  $[-h/2, h/2]$ , i.e.  
 47  $S = \Omega \times [-h/2, h/2]$ .

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

49 (1) 
$$\Delta u + \kappa^2 \epsilon(\mathbf{s}) u = 0 \quad \text{for all } \mathbf{s} \in \mathbb{R}^3$$

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

55 (2) 
$$\frac{\partial u^s}{\partial r} - i\kappa u^s = o(1/r), \quad r = \|\mathbf{s}\|.$$

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

58 Since we are considering the setting of two dimensional photonic crystal struc-  
 59 tures in a three dimensional scattering inhomogeneity, the refractive index is constant  
 60 in the direction of the thin component direction. We adapt the convention of Moskow  
 61 et. al. [13], where we write that the refractive index is represented by  $\epsilon_0(\mathbf{x})/h$ , where  
 62  $h$  is the length of the thin side. While refractive indices are material properties that  
 63 do not depend on size, high refraction indices are necessary to sufficiently reduce the  
 64 wavelength on the order of the length of the waveguide in the thin direction. Thus  
 65 we define the refractive index function

66 (3) 
$$\epsilon(\mathbf{x}, z) = \begin{cases} 1 & \text{for } (\mathbf{x}, z) \notin S; \\ \frac{\epsilon_0(\mathbf{x})}{h} & \text{for } (\mathbf{x}, z) \in S, \end{cases}$$

67 where  $\epsilon_0$  is compactly supported on  $\Omega$ . If  $u = u^s + u^i$  satisfies equations (1) and (2),  
 68 then  $u$  is also a solution to the Lippmann-Schwinger volume integral equation [5]

69 (4) 
$$u(\mathbf{s}) + \kappa^2 \int_S \left( 1 - \frac{\epsilon_0(\mathbf{x}')}{h} \right) G(\mathbf{s}, \mathbf{s}') u(\mathbf{s}') d\mathbf{s}' = u^i(\mathbf{s}),$$

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

72 (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  $\Omega$  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

$$u(\mathbf{x}, z) + \kappa^2 \int_{\Omega} \int_{-h/2}^{h/2} \left( 1 - \frac{\epsilon_0(\mathbf{x}')}{h} \right) G((\mathbf{x}, z), (\mathbf{x}', z')) u(\mathbf{x}', z') dz' d\mathbf{x}' = u^i(\mathbf{x}, z),$$

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

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

73 We write this compactly as

$$74 \quad (6) \quad (I + K)u(\mathbf{x}, \zeta) = u^i(\mathbf{x}, h\zeta),$$

75 where

$$76 \quad (7) \quad (Ku)(\mathbf{x}, \zeta) := \kappa^2 \int_{\Omega} \int_{-1/2}^{1/2} (h - \epsilon_o(\mathbf{x}')) G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta')) u(\mathbf{x}', \zeta') d\zeta' d\mathbf{x}'.$$

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

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

$$90 \quad (8) \quad \|r_m\| = \min_{u \in \mathcal{K}_m(A, u^i)} \|u^i - Au\|,$$

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

$$100 \quad \|r_m\| = \min_{p_m \in \mathcal{P}_m^0} \|p_m(A)u^i\|,$$

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

103 In practice, when the GMRES method is applied to the discretized linear system,  
104 an orthogonal basis for the approximating space is generated by the Arnoldi iteration  
105 [16], therefore the cost per iteration and memory requirements grows with each iteration  
106 as more memory is needed to record the basis for the growing Krylov subspace.  
107 Thus, GMRES, is feasible if the number of iterations remain small. However GMRES  
108 is too computationally expensive for this problem without effective preconditioning.

109 This is where we utilize the asymptotic results of [13] as a guide to building an  
 110 effective preconditioning scheme. That is, rather than apply GMRES to equation (6),  
 111 we solve the equivalent problem

$$112 \quad (AA_0^{-1})(A_0u) = u^i,$$

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

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

$$124 \quad (9) \quad (I - K_{2D})u_0(\mathbf{x}) = u^i(\mathbf{x}, 0)$$

125 where

$$126 \quad (10) \quad (K_{2D}u_0)(\mathbf{x}) := \kappa^2 \int_{\Omega} \epsilon_o(\mathbf{x}') G((\mathbf{x}, 0), (\mathbf{x}', 0)) u_0(\mathbf{x}') d\mathbf{x}'.$$

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

$$131 \quad (11) \quad (K_0u)(\mathbf{x}, \eta) = K_{2D} \left( \int_{-1/2}^{1/2} u(\mathbf{x}, \eta) d\eta \right)$$

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

136 **2.1. Solving the Preconditioning Step as a two dimensional system.** As  
 137 mentioned before, the right hand side data for the preconditioning operator  $A_0$  has  
 138 no physical interpretation, nor is it necessarily constant in the direction of the third  
 139 component. Furthermore, for such a system  $(A_0y)(s) = z(s)$ , the solution  $y(s)$  need  
 140 not be constant in the third component direction. However, this preconditioner, is  
 141 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

$$(K_0y)(\mathbf{s}) = y(\mathbf{s}) - z(\mathbf{s}).$$

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

$$144 \quad \kappa^2 \int_{\Omega} \int_{-1/2}^{1/2} \epsilon(\mathbf{x}') G((\mathbf{x}, 0), (\mathbf{x}', 0)) y(\mathbf{x}', \zeta') d\zeta' d\mathbf{x}' = \int_{-1/2}^{1/2} y(\mathbf{x}, \zeta') - z(\mathbf{x}, \zeta') d\zeta',$$

145 which can be rearranged to be

$$146 \quad \int_{-1/2}^{1/2} y(\mathbf{x}, \zeta') d\zeta' - \kappa^2 \int_{\Omega} \epsilon(\mathbf{x}') G((\mathbf{x}, 0), (\mathbf{x}', 0)) \left( \int_{-1/2}^{1/2} y(\mathbf{x}', \zeta') d\zeta' \right) d\mathbf{x}' = \int_{-1/2}^{1/2} z(\mathbf{x}, \zeta') d\zeta'$$

147 Define

$$148 \quad y_a(\mathbf{x}) = \int_{-1/2}^{1/2} y(\mathbf{x}, \zeta') d\zeta'$$

$$149 \quad z_a(\mathbf{x}) = \int_{-1/2}^{1/2} z(\mathbf{x}, \zeta') d\zeta'$$

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

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

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

$$151 \quad y(\mathbf{x}, \zeta) = \kappa^2 \int_{\Omega} \epsilon(\mathbf{x}') G((\mathbf{x}, 0), (\mathbf{x}', 0)) y_a(\mathbf{x}') d\mathbf{x}' + z(\mathbf{x}, \zeta)$$

$$152 \quad = y_a(\mathbf{x}) - z_a(\mathbf{x}) + z(\mathbf{x}, \zeta)$$

153 **3. Asymptotic Results.** We present here the main result from Moskow, et. al.  
154 [13] and extend it to obtain GMRES convergence bounds when applied to equations  
155 (9) and (10).

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

$$158 \quad \sup_{(\mathbf{x}, \zeta) \in \bar{S}} \int_{\Omega} |G((\mathbf{x}, 0), (\mathbf{x}', 0)) - G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta'))| d\mathbf{x}' < Ch$$

159

160 *Proof.* See Moskow, et. al. [13, Lemma 1]

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

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

$$168 \quad \|I - AA_0^{-1}\|_{L^\infty(\bar{S})} < C'h$$

169

*Proof.*

$$170 \quad \|I - AA_0^{-1}\| = \|(A_0 - A)A_0^{-1}\|$$

$$171 \quad \leq \|A_0^{-1}\| \|A_0 - A\|$$

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

$$173 \|A - A_0\| = \sup_{\|u\|=1} \|A_0 u - A u\|$$

$$174 = \sup_{\|u\|=1} \|K_o u + Ku\|$$

$$175 \leq \sup_{\|u\|=1} \sup_{(\mathbf{x}, \zeta) \in \bar{S}} \left( h\kappa^2 \int_{-1/2}^{1/2} \int_{\Omega} |G((\mathbf{x}, 0), (\mathbf{x}', 0))| |u(s')| ds' \right.$$

$$176 + h\kappa^2 \int_{-1/2}^{1/2} \int_{\Omega} |G((\mathbf{x}, 0), (\mathbf{x}', 0)) - G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta'))| |u(\mathbf{x}', \zeta')| d\zeta' d\mathbf{x}'$$

$$177 \left. + \kappa^2 \int_{-1/2}^{1/2} \int_{\Omega} \epsilon_0(\mathbf{x}') |G((\mathbf{x}, 0), (\mathbf{x}', 0)) - G((\mathbf{x}, h\zeta), (\mathbf{x}', h\zeta'))| |u(\mathbf{x}', \zeta')| d\zeta' d\mathbf{x}' \right)$$

$$178 \leq h\kappa^2 \left( \frac{M}{4\pi} + Ch + C\|\epsilon_0\|_{L^\infty(\Omega)} \right)$$

179 Therefore  $\|I - AA_0^{-1}\|$  is small if the scattering medium is sufficiently thin. However,  
180 note that this bound contains the constant  $\|A_0^{-1}\|$ , which, while independent of  $h$ ,  
181 could possibly be very large. However, in practice we see that  $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0\|$  is much  
182 smaller than the bounds we demonstrate in this corollary, where  $\mathbf{A}$ , and  $\mathbf{A}_0$  are  
183 discretizations of  $A$  and  $A_0$  respectively, using a collocation method we describe in  
184 section 4. We show this in figure 1.

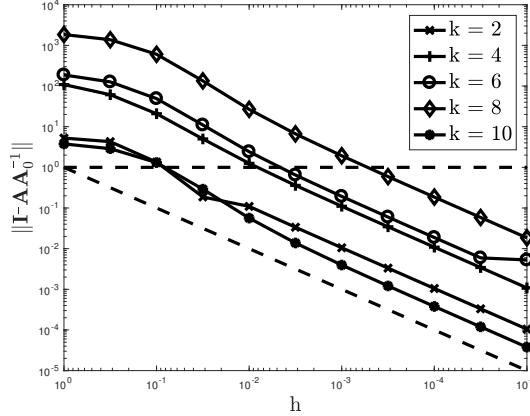


FIG. 1. Here we illustrate numerically the results of Corollary 2: that  $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\| = \mathcal{O}(h)$  (for  $\epsilon_0 = 1$ ). The horizontal dashed line is at 1 and the sloped dashed line is  $h$ .

185 The reason we do better is that by factoring out the inverse of the preconditioning  
186 operator  $A_0$ , we don't take into account spectral deflating. That is, we show in  
187 corollary 3, that  $\sigma(A) \in \sigma_\epsilon(A_0)$ , for  $\epsilon = O(h)$ . Thus the spectrum of  $A_0$  approximates  
188 the spectrum of  $A$ . Then the intuition we gain from the numerical results in figure 1  
189 lead us to believe that we not only approximate well the eigenvalues but also those  
190 eigenmodes with low enough frequency that they have small dependence on the thin  
191 direction component (of course the eigenfunctions of  $A_0$  are constant in the thin  
192 direction). Indeed we show that  $\sigma(\mathbf{A}\mathbf{A}_0^{-1}) \rightarrow 1$  as  $h \rightarrow 0$  in figure 2.

193 COROLLARY 3. Let  $A = I + K$ , where the operator  $K$  is defined in (7) and

194  $A_0 = I - K_0$ , where  $K_0$  is defined in (11), then  $\sigma(A) \in \sigma_\epsilon(A_0)$ , where  $\epsilon = O(h)$ .  
 195

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

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

202 where  $C$  is the constant from theorem 1.

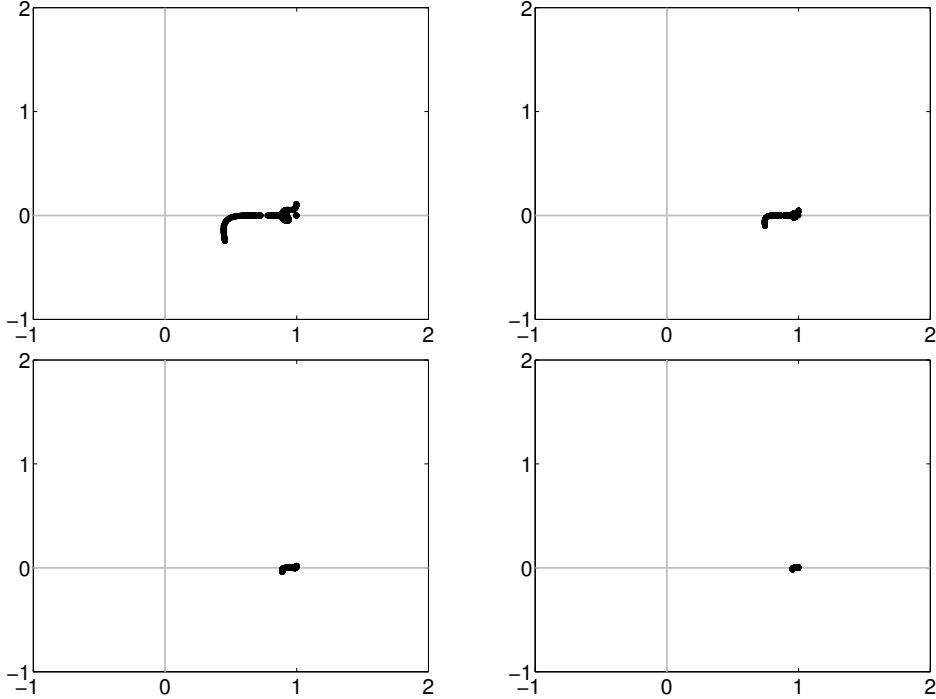


FIG. 2. The spectrum  $\sigma(\mathbf{A}\mathbf{A}_0^{-1})$  for values of  $h = 10^{-1}, 10^{-1.2}, 10^{-1.4}, 10^{-1.6}$  going left to right, top to bottom.

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

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

$$207 \quad (AA_0^{-1})(A_0u) = u^i,$$

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

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

$$211 \quad \|r_m\| \leq \min_{p_m \in \mathcal{P}_m^0} \|p_m(A)\| \|u^i\|$$

212 Then Corollary 2 implies that

$$213 \quad \frac{\|r_m\|}{\|u^i\|} \leq \|(I - AA_0^{-1})^m\| \\ 214 \quad \leq \|I - AA_0^{-1}\|^m \\ 215 \quad \leq \epsilon^m$$

216 where  $\epsilon = O(h)$ .

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

$$221 \quad \bar{G}(\mathbf{s}, \mathbf{s}') := \bar{G}((\mathbf{x}, \zeta), (\mathbf{x}, \zeta)') := G((\mathbf{x}, h\zeta), (\mathbf{x}, h\zeta)'), \\ 222 \quad \bar{u}^i(\mathbf{s}) := \bar{u}^i((\mathbf{x}, \zeta)) := u^i((\mathbf{x}, h\zeta)).$$

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

$$225 \quad G_0(\mathbf{s}, \mathbf{s}') := G((\mathbf{x}, 0), (\mathbf{x}', 0)) \\ 226 \quad u_0^i(\mathbf{s}) := u^i((\mathbf{x}, 0)).$$

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

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

$$237 \quad (\mathbf{I} - \mathbf{K})\mathbf{u} = \mathbf{u}^i$$

238 where

$$239 \quad \mathbf{K}_{ij} = \kappa^2 \int_{d_j} (h - \epsilon(\mathbf{s}')) \bar{G}(\mathbf{s}_i, \mathbf{s}') d\mathbf{s}' \\ 240 \quad \mathbf{u}_i^i = \bar{u}^i(\mathbf{s}_i)$$

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

242 **4.1. Solving the Preconditioned system.** Applying the same collocation  
 243 method to the preconditioner operator  $A_0 = I - K_0$ , we get a preconditioning matrix

244 
$$\mathbf{I} - \mathbf{K}_0$$

245 where

246 
$$(\mathbf{K}_0)_{ij} = \kappa^2 \int_{d_j} \epsilon(\mathbf{s}') G_0(\mathbf{s}_i, \mathbf{s}') d\mathbf{s}'$$

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

250 (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

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

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

$$(\mathbf{K}_{2D})_{ij} = \kappa^2 \int_{\omega_j} \epsilon_0(\mathbf{x}') G_0((\mathbf{x}_i, 0), (\mathbf{x}', 0)) d\mathbf{x}',$$

251 where  $\{\omega_j\}_{j=1}^n$  is a discretization of  $\Omega$  corresponding to the discretization of  $\Omega \times$   
 252  $[-1/2, 1/2]$  into  $\{d_j\}_{j=1}^n$ . The entries of  $\mathbf{K}_{2D}$  are approximated using Clenshaw Curtis  
 253 quadrature.

**4.2. Solving the discretized Preconditioner as a two dimensional problem.** The linear algebra analog 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  $\mathbf{z}$

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

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

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

254 Let

255 
$$\mathbf{y}_a = \frac{1}{m} \sum_{k=1}^m \mathbf{y}_k,$$

256 
$$\mathbf{z}_a = \frac{1}{m} \sum_{k=1}^m \mathbf{z}_k.$$

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

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

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

$$\begin{aligned} 258 \quad \mathbf{y}_k &= \mathbf{z}_k + \mathbf{K}_{2D}\mathbf{u}_a \\ 259 \quad &= \mathbf{z}_k - \mathbf{z}_a + \mathbf{y}_a \end{aligned}$$

260 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  
261 the  $m \times m$  matrix of all ones and  $\otimes$  is the Kronecker product.

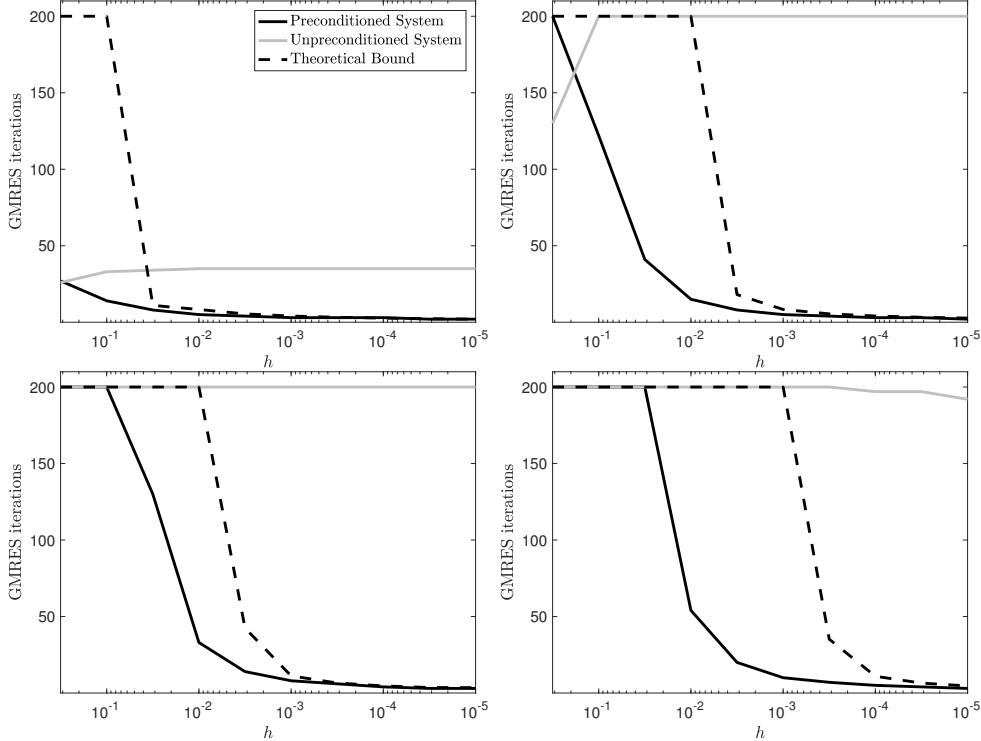


FIG. 3. GMRES Iteration counts as a function of  $h$  for  $k = 2, 4, 6, 8$  (left to right, top to bottom). The solid black line gives the iteration count for the preconditioned system. The solid grey line gives the iteration count for the unpreconditioned system. The maximum iteration was set to 200. 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 Matlab's `randn` function.

262 **5. Numerical Results.** To demonstrate the effectiveness of the preconditioning  
263 scheme presented in the previous section, we present the results of several numerical  
264 experiments in this section. For all problems in the section, the scattering obstacle is  
265 a square slab that is  $\kappa \times \kappa$  wavelengths with width  $h$ . That is, the scattering obstacle  
266  $S = \Omega \times [-h/2, h/2]$ , where  $\Omega$  is the  $2\pi \times 2\pi$  square. The grid used for discretization  
267 is  $24 \times 24 \times 7$ .

268 The number of Chebyshev nodes used to compute each matrix entry is  $3^2$  for the  
269 two dimensional grid and  $3^3$  for the three dimensional grid. The refractive index is

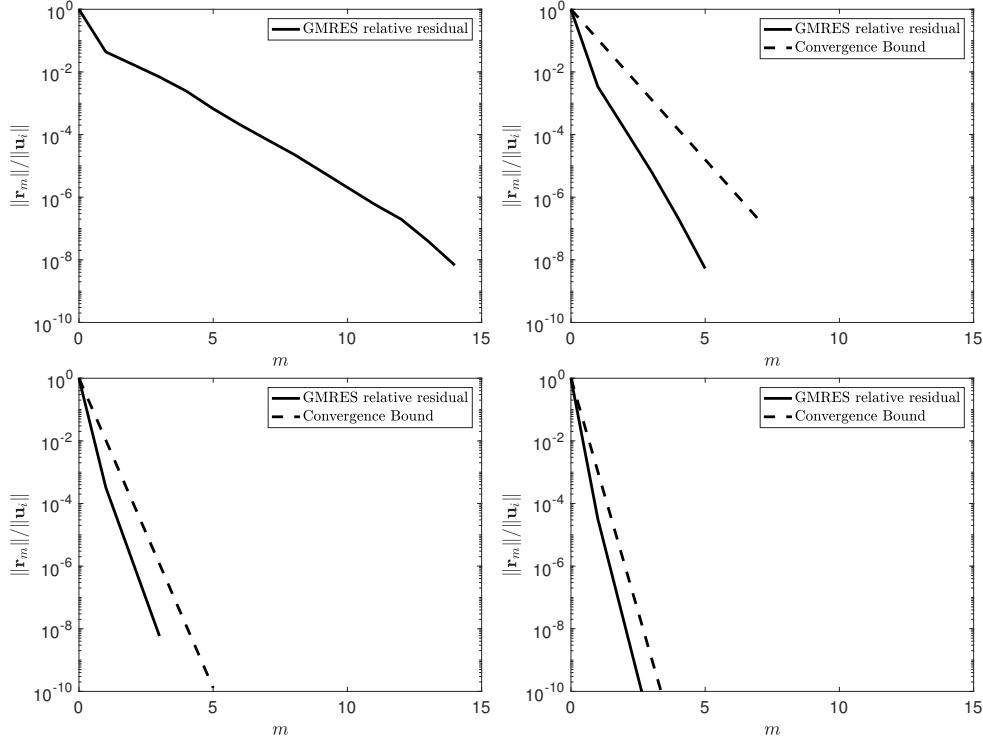


FIG. 4. For  $\kappa = 2$ ,  $\varepsilon_0 = 1$  and  $h = 10^{-1}, 10^{-2}, 10^{-3}$  left to right and top to bottom, we plot the relative residuals in the solid black line and, if applicable, the bound  $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2^m$  in a dashed line.

270 constant. Figure 4 illustrate the relative residual norm for the first ten iterates of the  
 271 GMRES method, as well as the bound for the residual  $\|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2^m$  at each iteration  
 272  $m$  if applicable.

273 GMRES shows considerable improved performance when applied to the precon-  
 274 ditioned system compared to the original discretized system for sufficiently thin in-  
 275 homogeneities. Figures 3 and 5 show that for values of  $h < 10^{-1}$  (and sometimes  
 276 for thicker inhomogeneities), we begin to get substantial reduction in the number  
 277 of GMRES iterations required for convergence. Furthermore, the numerical experi-  
 278 ments show that the bounds demonstrated in Corollary 4 are effective at predicting  
 279 the fast convergence for the preconditioned problem. The corollary suggests that  
 280 the number of iterations required for convergence can be bounded by  $\lceil \log_\varepsilon(\text{tol}) \rceil$  if  
 281  $\varepsilon := \|\mathbf{I} - \mathbf{A}\mathbf{A}_0^{-1}\|_2 < 1$ . In all the numerical experiments presented here, the tolerance  
 282 for the relative residual is set to  $\text{tol} = 10^{-8}$ .

Figure 5 illustrate 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 non constant and periodic and is given by

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

283 **6. Conclusion and Further Work.** Building thin, photonic band gap media  
 284 with two dimensional periodic structure is important to power and material reduction  
 285 [19]. Therefore the efficient computational modeling of time harmonic scattering

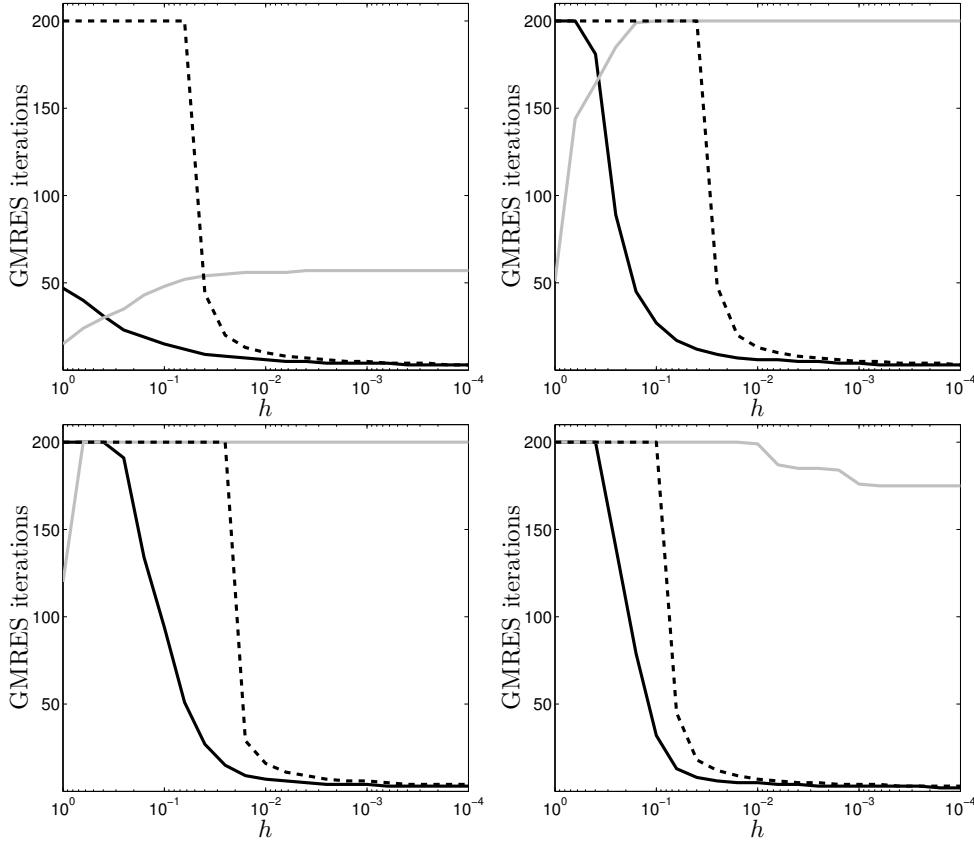


FIG. 5. GMRES Iteration counts as a function of  $h$  for  $k = 2, 4, 6, 8$  (left to right, top to bottom). The solid black line gives the iteration count for the preconditioned system. The solid grey line gives the iteration count for the unpreconditioned system. The maximum iteration was set to 200. 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  $\varepsilon_0(x_1, x_2) = 1 + |\sin(3x_1)\sin(3x_2)|$ .

through such media is useful to such applications to the field of optics. We have shown 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  $\mathcal{O}(N^2)$  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,

303 such an approach would have to align an efficient mesh configuration with the tiled  
 304 format demonstrated in (12). It is important to point out, however, that if one were  
 305 to employ a Nyström discretization, one would have to take care of vertically aligned,  
 306 but unequal, vertices of the mesh, since as  $h \rightarrow 0$ , the Green's function approaches a  
 307 singularity that wouldn't appear in the two dimensional discretization, implying that  
 308 our preconditioner no longer approximates an inverse. However, we are confident that  
 309 one can significantly accelerate the integral computations at a high order of accuracy  
 310 and combine such a method with the preconditioning method described in this paper  
 311 to produce a high order and efficient method for solving this problem. Such a result  
 312 would be a significant and welcome contribution.

## 313 REFERENCES

- 314 [1] O. BRUNO AND A. SEI, *A fast high-order solver for em scattering from complex penetrable*  
 315 *bodies: Te case*, Antennas and Propagation, IEEE Transactions on, 48 (2000), pp. 1862–  
 316 1864.
- 317 [2] Z.-H. CAO, *A note on the convergence behavior of GMRES*, Appl. Num. Math., 25 (1997),  
 318 pp. 13–20.
- 319 [3] Y. CHEN, *A fast, direct algorithm for the lippmann-schwinger integral equation in two dimen-*  
 320 *sions.*, Advances in Computational Mathematics, 16 (2002), pp. 175–190.
- 321 [4] C. W. CLENSHAW AND A. R. CURTIS, *A method for numerical integration on an automatic*  
 322 *computer*, Numer. Math., 2 (1960), pp. 197–205.
- 323 [5] D. COLTON AND R. KRESS, *Inverse Acoustic and Electromagnetic Scattering Theory*, Springer-  
 324 Verlag, Berlin, 1998.
- 325 [6] S. FAN, J. WINN, A. DEVENYI, J. CHEN, R. MEADE, AND J. JOANNOPOULOS, *Guided and defect*  
 326 *modes in periodic waveguides*, J. Opt. Soc. Amer. B Opt. Phys., 12 (1995), pp. 1267–1283.
- 327 [7] L. GREENGARD AND V. ROKHLIN, *A fast algorithm for particle simulations*, Journal of Com-  
 328 *putational Physics*, 135 (1997), pp. 280 – 292.
- 329 [8] E. M. HYDE AND O. P. BRUNO, *An efficient, preconditioned, high-order solver for scattering*  
 330 *by two-dimensional inhomogeneous media*, J. Comp. Phys., 200 (2004), pp. 670–694.
- 331 [9] ———, *A fast, higher-order solver for scattering by penetrable bodies in three dimensions*, J.  
 332 *Comp. Phys.*, 202 (2005), pp. 236–261.
- 333 [10] C. JOHNSON, *Numerical Solution of Partial Differential Equations by the Finite Element*  
 334 *Method*, Cambridge University Press, Sweden, 1995.
- 335 [11] E. KREYSZIG, *Introductory Functional Analysis with Applications*, Wiley, New York, 1989.
- 336 [12] I. MORET, *A note on the superlinear convergence of GMRES*, SIAM J. Num. Anal., 34 (1997),  
 337 pp. 513–516.
- 338 [13] S. MOSKOW, F. SANTOSA, AND J. ZHANG, *An approximate method for scattering by thin struc-*  
 339 *tures*, SIAM J. Appl Math., 66 (2005), pp. 187–205.
- 340 [14] K. NABORS, F. T. KORMEYER, F. T. LEIGHTON, AND J. WHITE, *Preconditioned, adaptive,*  
 341 *multipole-accelerated iterative methods for three-dimensional first-kind integral equations*  
 342 *of potential theory*, SIAM J. Sci. Comput., 15 (1994), pp. 713–735.
- 343 [15] V. ROKHLIN, *Rapid solution of integral equations of scattering theory in two dimensions*, Jour-  
 344 *nal of Computational Physics*, 86 (1990), pp. 414 – 439.
- 345 [16] Y. SAAD AND M. H. SCHULTZ, *GMRES: A generalized minimal residual algorithm for solving*  
 346 *nonsymmetric linear systems*, SIAM J. Sci. Stat. Comp., 7 (1986), pp. 856–869.
- 347 [17] J. SIFUENTES, *Preconditioning the integral formulation of the helmholtz equation via deflation*,  
 348 Master's thesis, Rice University, 2006.
- 349 [18] V. SIMONCINI AND D. B. SZYLD, *On the occurrence of superlinear convergence of exact and*  
 350 *inexact Krylov subspace methods*, SIAM Review, 47 (2005), pp. 247–272.
- 351 [19] P. VILLENEUVE, S. FAN, S. JOHNSON, AND J. JOANNOPOULOS, *Three-dimensional photon con-*  
 352 *finement in photonic crystals of low-dimensional periodicity*, IEE Proc. Optoelectron, 145  
 353 (1998), pp. 384–390.
- 354 [20] J. VUCKOVIC, M. LONCAR, H. MABUCHI, AND A. SCHERER, *Optimization of the q factor in*  
 355 *photonic crystal microwavities*, IEEE J. Quantum Elec., 38 (2002), pp. 850–856.
- 356 [21] R. WINTHER, *Some superlinear convergence results for the conjugate gradient method*, SIAM  
 357 *J. Num. Anal.*, 17 (1980), pp. 14–17.