

A CARTESIAN PERFECTLY MATCHED LAYER FOR THE HELMHOLTZ EQUATION

SEMYON TSYNKOV* AND ELI TURKEL †

Abstract. We consider the two-dimensional scalar Helmholtz equation in an unbounded (in at least one direction) domain. To implement this on a computer it is necessary to truncate the infinite domain and to introduce an artificial boundary. In order to minimize reflections we introduce a PML layer that damps the waves outside the physical domain.

We analyze the solvability, uniqueness and limit properties for several different formulations of the PML model. We consider finite domains filled with PML, the PML equations on the entire plane, combined vacuum–PML problem on the entire plane, and combined vacuum–PML problem in a waveguide. We consider both an infinitely thick PML and a PML of finite thickness, in the latter case we analyze the reflection properties. The tools for the analysis of the foregoing problems are energy-type estimates and separation of variables.

We also consider numerical approximations. We construct a fourth order accurate approximation to the Helmholtz equation. Allowing the non-differentiated term to vary with x and y presents no difficulties to the high order scheme. However, the variable coefficients multiplying the derivatives do not allow a higher order implementation. On the other hand, the order of accuracy in the PML layer is irrelevant since it is an artificial device. The important matter is to prevent reflections rather than have higher accuracy. We also discuss iterative methods and preconditioning for solving the Helmholtz and PML equations.

1. Introduction. Berenger [4,5] introduced the PML (Perfectly Matched Layer) as a way of absorbing waves at artificial surfaces for the time dependent Maxwell equations. Abarbanel and Gottlieb later showed [1] that Berenger’s approach was not well posed and several other approaches have since been suggested. In [18] we showed that several of these approaches including those of Ziolkowsky [20] and Gedney [7] are linearly equivalent. We present the three dimensional PML equations in a form similar to that of [7,19].

Let \vec{E} and \vec{H} be the electric and magnetic vectors. We introduce \vec{B} and \vec{D} as artificial variables that are not related to any physical quantities. These have been nondimensionalized for convenience. The UPML is then given by:

$$\begin{aligned}
 \frac{\partial D_x}{\partial t} + \sigma_y D_x &= \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} & \frac{\partial B_x}{\partial t} + \sigma_y B_x &= \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \\
 \frac{\partial D_y}{\partial t} + \sigma_z D_y &= \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} & \frac{\partial B_y}{\partial t} + \sigma_z B_y &= \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \\
 \frac{\partial D_z}{\partial t} + \sigma_x D_z &= \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} & \frac{\partial B_z}{\partial t} + \sigma_x B_z &= \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \\
 \frac{\partial D_x}{\partial t} + \sigma_x D_x &= \frac{\partial E_x}{\partial t} + \sigma_z E_x & \frac{\partial B_x}{\partial t} + \sigma_x B_x &= \frac{\partial H_x}{\partial t} + \sigma_z H_x \\
 \frac{\partial D_y}{\partial t} + \sigma_y D_y &= \frac{\partial E_y}{\partial t} + \sigma_x E_y & \frac{\partial B_y}{\partial t} + \sigma_y B_y &= \frac{\partial H_y}{\partial t} + \sigma_x H_y \\
 \frac{\partial D_z}{\partial t} + \sigma_z D_z &= \frac{\partial E_z}{\partial t} + \sigma_y E_z & \frac{\partial B_z}{\partial t} + \sigma_z B_z &= \frac{\partial H_z}{\partial t} + \sigma_y H_z
 \end{aligned} \tag{1.1}$$

σ_x is a function only of x and similarly for σ_y, σ_z . Thus, in any one direction only one of the σ is different from zero. It is only in the corners that more than one σ can be non-zero. For the theory one usually assumes that each σ is piecewise constant and so they are discontinuous at the interface of the physical domain and the PML. For numerical purposes the σ are chosen as differentiable functions.

We reduce this to two dimensions and change notation to acoustics. Let (p, u, v) be the physical variables

* School of Mathematical Sciences, Tel Aviv University, Ramat Aviv, Tel Aviv 69978, ISRAEL. E-mail: tsynkov@math.tau.ac.il, URL: <http://www.math.tau.ac.il/~tsynkov/>.

† School of Mathematical Sciences, Tel Aviv University, Ramat Aviv, Tel Aviv 69978, ISRAEL. E-mail: turkel@math.tau.ac.il, URL: <http://www.math.tau.ac.il/~turkel/>.

and (P, U, V) be artificial variables. Then we get

$$\begin{aligned} P_t + \sigma_x P &= c(u_x + v_y) \\ P_t &= p_t + \sigma_y p \\ U_t &= cp_x \\ U_t + \sigma_y U &= u_t + \sigma_x u \\ V_t + \sigma_y V &= cp_y \\ V_t + \sigma_x V &= v_t \end{aligned}$$

Fourier transforming in time and eliminating the artificial variables results in the following system:

$$\begin{aligned} i\omega s_x s_y p &= c(u_x + v_y) \\ i\omega \frac{s_x}{s_y} u &= cp_x \\ i\omega \frac{s_y}{s_x} v &= cp_y \end{aligned} \tag{1.2}$$

where

$$s_x = 1 + \frac{\sigma_x}{i\omega}, \quad s_y = 1 + \frac{\sigma_y}{i\omega}. \tag{1.3}$$

We convert this to a second order equation (see [18]) for p . For convenience we shall label the solution as u rather than the physical variable p .

$$\mathbf{L}u \equiv \frac{\partial}{\partial x} \left(\frac{s_y}{s_x} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{s_x}{s_y} \frac{\partial u}{\partial y} \right) + s_x s_y \omega^2 u = 0, \tag{1.4}$$

The quantities σ_x and σ_y are real and non-negative, $\sigma_x \geq 0$ and $\sigma_y \geq 0$. In the areas where at least one of these quantities is positive, $\sigma_x > 0$ or $\sigma_y > 0$, the equation attenuates traveling waves. In the areas where both $\sigma_x = 0$ and $\sigma_y = 0$ this reduces to the Helmholtz equation:

$$\Delta u + \omega^2 u = 0. \tag{1.5}$$

2. Theoretical Foundations. We will study the solvability and uniqueness of the Helmholtz PML equation in Cartesian coordinates. For the rest of this section, we will assume for simplicity that σ_x and σ_y of (1.3) are piece-wise constant functions and specifically, they are zero inside the physical domain and each equal to a (non-zero) constant in the PML layer. This assumption simplifies the analysis and at the same time does not present any significant limitations, as it can be alleviated at a later stage. The piece-wise constant character of the coefficients implies that for any particular problem that combines both the areas of vacuum (1.5) and PML (1.4), special boundary conditions have to be set at the interfaces between different areas. These boundary conditions are standard for elliptic equations with discontinuous coefficients, i.e., continuity of the solution and its normal flux across the interface. A particular formulation of the interface conditions will be discussed later on, see Section 2.3.

2.1. Uniqueness on a Bounded Domain. The solution to the Helmholtz equation (1.5) on a bounded domain, in particular, solution to the Dirichlet boundary-value problem, may be non-unique. This happens when ω^2 of (1.5) is an eigenvalue of the corresponding Laplacian boundary-value problem. The following theorem implies that there exists no more than one solution of equation 1.4 on a bounded domain Ω with the Dirichlet boundary conditions.

THEOREM 2.1. *Let $\Omega \subset \mathbb{R}^2$ be a bounded domain and $u = u(x, y)$, $(x, y) \in \Omega$, satisfy equation (1.4) with the Dirichlet boundary condition $u|_{\partial\Omega} = 0$. Then, $u(x, y) \equiv 0$, $(x, y) \in \Omega$.*

Proof. Let \bar{u} be the complex conjugate of u . Using the energy method we have

$$\begin{aligned}
\int_{\Omega} \bar{u} \mathbf{L}u \, d\Omega &= \int_{\Omega} \left[\bar{u} \frac{\partial}{\partial x} \left(\frac{s_y}{s_x} \frac{\partial u}{\partial x} \right) + \bar{u} \frac{\partial}{\partial y} \left(\frac{s_x}{s_y} \frac{\partial u}{\partial y} \right) + s_x s_y \omega^2 |u|^2 \right] d\Omega = \\
&= \int_{\Omega} \left[\frac{\partial}{\partial x} \left(\frac{s_y}{s_x} \bar{u} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{s_x}{s_y} \bar{u} \frac{\partial u}{\partial y} \right) + s_x s_y \omega^2 |u|^2 \right] d\Omega - \int_{\Omega} \left[\frac{s_y}{s_x} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{s_x}{s_y} \left| \frac{\partial u}{\partial y} \right|^2 \right] d\Omega = \\
&= \int_{\partial\Omega} \left[\frac{s_y}{s_x} \bar{u} \frac{\partial u}{\partial x} n_x + \frac{s_x}{s_y} \bar{u} \frac{\partial u}{\partial y} n_y \right] dl - \int_{\Omega} \left[\frac{s_y}{s_x} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{s_x}{s_y} \left| \frac{\partial u}{\partial y} \right|^2 - s_x s_y \omega^2 |u|^2 \right] d\Omega,
\end{aligned}$$

here n_x and n_y are the Cartesian components of the outward normal \mathbf{n} to the boundary $\partial\Omega$ and dl is the element of the arc length along $\partial\Omega$. The first integral is equal zero because $\bar{u}|_{\partial\Omega} = 0$. Since $u(x, y)$ is a solution of (1.4) on Ω , we obtain

$$\int_{\Omega} \left[\frac{s_y}{s_x} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{s_x}{s_y} \left| \frac{\partial u}{\partial y} \right|^2 - s_x s_y \omega^2 |u|^2 \right] d\Omega = 0. \quad (2.1a)$$

Dividing equation (2.1a) by $s_x s_y$, which is a constant across Ω , we find that

$$\int_{\Omega} \left[\frac{1}{s_x^2} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{1}{s_y^2} \left| \frac{\partial u}{\partial y} \right|^2 - \omega^2 |u|^2 \right] d\Omega = 0. \quad (2.1b)$$

Both the real and imaginary part of the left-hand side of (2.1b) must separately equal to zero. Using (1.3), this yields for the imaginary part:

$$\Im \int_{\Omega} \left[\frac{1}{s_x^2} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{1}{s_y^2} \left| \frac{\partial u}{\partial y} \right|^2 - \omega^2 |u|^2 \right] d\Omega = \int_{\Omega} \left[\frac{2\sigma_x \omega^3}{(\sigma_x^2 + \omega^2)^2} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{2\sigma_y \omega^3}{(\sigma_y^2 + \omega^2)^2} \left| \frac{\partial u}{\partial y} \right|^2 \right] d\Omega = 0. \quad (2.2)$$

From (2.2) we conclude that as long as σ_x and σ_y are of the same sign and are non-zero, $\nabla u \equiv 0$ on the entire Ω , which means $u(x, y) \equiv \text{const}$, $(x, y) \in \Omega$. From the homogeneous Dirichlet boundary condition it then immediately follows that $u(x, y) \equiv 0$, $(x, y) \in \Omega$. \square

In applications, the PML equations of type (1.4) are most often used for rectangular geometries.

PROPOSITION 2.2. *Let $\Omega \subset \mathbb{R}^2$ be a rectangular domain with its sides aligned with the Cartesian directions x and y , and $u = u(x, y)$, $(x, y) \in \Omega$, satisfy equation (1.4) and a general Robin boundary condition $\alpha u + \beta \frac{\partial u}{\partial \mathbf{n}}|_{\partial\Omega} = 0$; where $\alpha = \alpha(l) \in \mathbb{R}$ and $\beta = \beta(l) \in \mathbb{R}$ are real functions, $\alpha \geq 0$, $\beta > 0$. Then, $u(x, y) \equiv 0$, $(x, y) \in \Omega$.*

Proof. We repeat the steps of the proof of Theorem 2.1.

$$\int_{\Omega} \bar{u} \mathbf{L}u \, d\Omega = \int_{\partial\Omega} \left[\frac{s_y}{s_x} \bar{u} \frac{\partial u}{\partial x} n_x + \frac{s_x}{s_y} \bar{u} \frac{\partial u}{\partial y} n_y \right] dl - \int_{\Omega} \left[\frac{s_y}{s_x} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{s_x}{s_y} \left| \frac{\partial u}{\partial y} \right|^2 - s_x s_y \omega^2 |u|^2 \right] d\Omega.$$

Since Ω is a Cartesian rectangle, we can rewrite the first integral on the right-hand side of the previous equality using the fact that for the x -aligned sides of the rectangle $dl = dx$, $n_x = 0$, and $n_y = \pm 1$, and for its y -aligned sides $dl = dy$, $n_x = \pm 1$, and $n_y = 0$. We also take into account that when $n_x = 0$ and $n_y = \pm 1$, the original Robin boundary condition reduces to $\alpha u \pm \beta \frac{\partial u}{\partial y} = 0$, respectively; and for $n_x = \pm 1$, $n_y = 0$ it reduces to $\alpha u \pm \beta \frac{\partial u}{\partial x} = 0$, respectively. Thus, using that $\mathbf{L}u = 0$ we obtain

$$-\int_{\partial\Omega} \frac{s_x}{s_y} \frac{\alpha}{\beta} |u|^2 dx - \int_{\partial\Omega} \frac{s_y}{s_x} \frac{\alpha}{\beta} |u|^2 dy - \int_{\Omega} \left[\frac{s_y}{s_x} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{s_x}{s_y} \left| \frac{\partial u}{\partial y} \right|^2 - s_x s_y \omega^2 |u|^2 \right] d\Omega = 0. \quad (2.3)$$

Splitting the imaginary and real parts in (2.3) as before, we get:

$$\begin{aligned} & \int_{\partial\Omega} \frac{2\sigma_y \omega^3}{(\sigma_y^2 + \omega^2)^2} \frac{\alpha}{\beta} |u|^2 dx + \int_{\partial\Omega} \frac{2\sigma_x \omega^3}{(\sigma_x^2 + \omega^2)^2} \frac{\alpha}{\beta} |u|^2 dy + \\ & + \int_{\Omega} \left[\frac{2\sigma_x \omega^3}{(\sigma_x^2 + \omega^2)^2} \left| \frac{\partial u}{\partial x} \right|^2 + \frac{2\sigma_y \omega^3}{(\sigma_y^2 + \omega^2)^2} \left| \frac{\partial u}{\partial y} \right|^2 \right] d\Omega = 0. \end{aligned} \quad (2.4)$$

From (2.4) we see that both $\nabla u \equiv 0$, $(x, y) \in \Omega$, and $u|_{\partial\Omega} = 0$. This implies the desired statement. \square

A typical configuration of the problem solved numerically with the help of the PML methodology includes a rectangular computational domain surrounded by the PML of a finite thickness. As a rule, inside the PML $\sigma_x = 0$ for the x -aligned portions of the layer, and $\sigma_y = 0$ for its y -aligned portions.

PROPOSITION 2.3. *Let $\Omega \subset \mathbb{R}^2$ be a rectangular domain with its sides aligned with the Cartesian directions x and y , and $u = u(x, y)$, $(x, y) \in \Omega$, satisfy equation (1.4) with $s_y \equiv 1$ and Dirichlet boundary condition $u|_{\partial\Omega} = 0$. Then, $u(x, y) \equiv 0$, $(x, y) \in \Omega$.*

Proof. We again repeat the steps of the proof of Theorem 2.1. Taking into account that $s_y \equiv 1$, we obtain instead of (2.2):

$$\Im \int_{\Omega} \left[\frac{1}{s_x^2} \left| \frac{\partial u}{\partial x} \right|^2 + \left| \frac{\partial u}{\partial y} \right|^2 - \omega^2 |u|^2 \right] d\Omega = \int_{\Omega} \frac{2\sigma_x \omega^3}{(\sigma_x^2 + \omega^2)^2} \left| \frac{\partial u}{\partial x} \right|^2 d\Omega = 0. \quad (2.5)$$

From (2.5) we conclude that $\partial u / \partial x \equiv 0$ across the entire Ω , which implies that $u(x, y) = u(y)$ or in other words, $u(x, y) = \text{const}$ along every line parallel to the x -axis. Since every line of this kind intersects the y -aligned sides of Ω , and the values of u at these intersection points are zero because of the homogeneous Dirichlet boundary condition $u|_{\partial\Omega} = 0$, we obtain that $u(x, y) = 0$ along every line parallel to the x -axis and therefore, $u(x, y) \equiv 0$, $(x, y) \in \Omega$. \square

REMARK 2.4. *A result similar to the one of Proposition 2.3 holds for $s_x \equiv 1$.*

The extension of these proofs to three dimensions is straightforward.

2.2. Solvability and Uniqueness on the Entire Plane. It is known that the solution to the Helmholtz equation (1.5) on an unbounded domain, in particular, on the entire \mathbb{R}^2 , is not determined uniquely by only requiring that it vanish or be bounded at infinity. To guarantee uniqueness, one typically needs some additional conditions at ‘‘infinity.’’ These are usually expressed as a requirement that all waves at infinity be outgoing, which, in turn, requires a definition of incoming and outgoing waves. For the time-dependent wave equation it is obvious what is meant by incoming and outgoing waves. However, the Helmholtz equation is obtained by a Fourier transform, in time, of the wave equation. Accordingly, the definition of incoming/outgoing in the Fourier domain depends on the definition of the Fourier transform, i.e., whether $e^{i\omega t}$ is used or $e^{-i\omega t}$. Thus, considering for simplicity the one-dimensional case first, we conclude that in the Helmholtz framework one can define outgoing waves for $x \rightarrow +\infty$ as those that behave as either $e^{i\omega x}$ or $e^{-i\omega x}$, where the sign is arbitrary; it is only required that one be consistent. (Note, in 1D for $x \rightarrow -\infty$ the signs will reverse.) In this paper we shall define, as is usual in electromagnetics, an outgoing wave as $e^{-i\omega x}$. Accordingly, σ_x (and σ_y) in (1.4) are required to be positive, because in this case consistently with the definition of the Fourier transform, the PML equation attenuates traveling waves, see below. Switching the definition of outgoing waves would require that σ_x (and σ_y) be negative. Hence, if σ_x and σ_y are considered functions of ω they must be even functions.

In the two-dimensional case the additional conditions specified as $r \equiv \sqrt{x^2 + y^2} \rightarrow \infty$ in order to guarantee uniqueness are known as the Sommerfeld radiation conditions:

$$u = O(r^{-1/2}), \quad (2.6a)$$

$$\frac{\partial u}{\partial r} + i\omega u = o(r^{-1/2}). \quad (2.6b)$$

Boundary conditions (2.6) guarantee that the solution at infinity be composed of the outgoing waves only. Similarly to the one-dimensional case mentioned previously, the sign in front of $i\omega u$ depends on the definition of an outgoing wave. The fundamental solution of the Helmholtz operator with boundary conditions 2.6, i.e., the solution to the non-homogeneous equation

$$\Delta \mathcal{E}_0 + \omega^2 \mathcal{E}_0 = \delta, \quad (2.7)$$

where δ is Dirac's measure at 0, is given by the Hankel function

$$\mathcal{E}_0 = \frac{\pi}{2i} H_0^{(2)}(\omega r). \quad (2.8)$$

In contradistinction to the Helmholtz equation (1.5), one does not need any special radiation conditions at infinity, like conditions (2.6), to ensure the solvability and uniqueness for the PML equation (1.4). Let us introduce the Schwartz space of test functions $\mathcal{D}(\mathbb{R}^2)$ that consists of all compactly supported infinitely differentiable functions on \mathbb{R}^2 and the space of distributions $\mathcal{D}'(\mathbb{R}^2)$, which is a conjugate space to $\mathcal{D}(\mathbb{R}^2)$, i.e., the space of all linear continuous functionals over $\mathcal{D}(\mathbb{R}^2)$. Along with $\mathcal{D}(\mathbb{R}^2)$ and $\mathcal{D}'(\mathbb{R}^2)$, we also consider the space of test functions $\mathcal{S}(\mathbb{R}^2)$ that contains all infinitely differentiable functions on \mathbb{R}^2 that for large values of the argument decay with all their derivatives faster than any power of $r^{-1} = (x^2 + y^2)^{-1/2}$, and the space of tempered distributions $\mathcal{S}'(\mathbb{R}^2)$, which is a conjugate space to $\mathcal{S}(\mathbb{R}^2)$, i.e., the space of all continuous linear functionals over $\mathcal{S}(\mathbb{R}^2)$. Clearly, $\mathcal{D}(\mathbb{R}^2) \subset \mathcal{S}(\mathbb{R}^2)$ and consequently, $\mathcal{S}'(\mathbb{R}^2) \subset \mathcal{D}'(\mathbb{R}^2)$.

THEOREM 2.5. *Let $f \in \mathcal{D}'(\mathbb{R}^2)$ be a compactly supported distribution. Then, the equation*

$$\frac{\partial}{\partial x} \left(\frac{s_y}{s_x} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{s_x}{s_y} \frac{\partial u}{\partial y} \right) + s_x s_y \omega^2 u = f \quad (2.9)$$

is solvable in the Schwartz space $\mathcal{D}'(\mathbb{R}^2)$.

Proof. We need to consider two different cases. First assume that both $\sigma_x \neq 0$ and $\sigma_y \neq 0$ (see (1.3)), i.e., both s_x and s_y are complex. By applying the Fourier transform technique, we obtain that the tempered fundamental solution of the differential operator \mathbf{L} of (1.4), i.e., the solution of equation

$$\frac{\partial}{\partial x} \left(\frac{s_y}{s_x} \frac{\partial \mathcal{E}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{s_x}{s_y} \frac{\partial \mathcal{E}}{\partial y} \right) + s_x s_y \omega^2 \mathcal{E} = \delta \quad (2.10)$$

in the Schwartz space $\mathcal{S}'(\mathbb{R}^2)$, $\mathcal{E} \in \mathcal{S}'(\mathbb{R}^2)$, is given by the inverse Fourier transform of the solution $F[\mathcal{E}] \in \mathcal{S}'(\mathbb{R}^2)$ of the following algebraic equation

$$P(\xi, \eta) F[\mathcal{E}] = 1. \quad (2.11)$$

In equation (2.11) and henceforth, $F[\cdot]$ denotes the Fourier transform over $\mathcal{S}'(\mathbb{R}^2)$, similarly, $F^{-1}[\cdot]$ will denote the inverse Fourier transform. $P(\xi, \eta)$ in (2.11) is the symbol of the operator \mathbf{L} of (1.4), i.e., the algebraic polynomial

$$P(\xi, \eta) = -\frac{s_y}{s_x} \xi^2 - \frac{s_x}{s_y} \eta^2 + s_x s_y \omega^2, \quad (2.12)$$

where ξ and η are the dual Fourier variables to x and y , respectively.

According to the general results of [10], equation (2.10) can always be solved in $\mathcal{S}'(\mathbb{R}^2)$ with respect to $F[\mathcal{E}]$ unless $P(\xi, \eta) \equiv 0$. For the specific $P(\xi, \eta)$ given by (2.12), it is particularly easy to explicitly construct the solution. First, we show that the polynomial $P(\xi, \eta)$ has no real zeros. Indeed, since we are looking for the real solutions of equation $P(\xi, \eta) = 0$, we divide both sides of this equation by $s_x s_y$ and arrive at the following algebraic system

$$\Im \left(\frac{P(\xi, \eta)}{s_x s_y} \right) \equiv -\omega^2 \left(\frac{2\sigma_x \omega}{(\sigma_x^2 + \omega^2)^2} \xi^2 + \frac{2\sigma_y \omega}{(\sigma_y^2 + \omega^2)^2} \eta^2 \right) = 0 \quad (2.13a)$$

$$\Re \left(\frac{P(\xi, \eta)}{s_x s_y} \right) \equiv \frac{\sigma_x^2 - \omega^2}{(\sigma_x^2 + \omega^2)^2} \xi^2 + \frac{\sigma_y^2 - \omega^2}{(\sigma_y^2 + \omega^2)^2} \eta^2 + 1 = 0 \quad (2.13b)$$

If $\sigma_x \neq 0$, $\sigma_y \neq 0$ and $\omega \neq 0$, then (2.13a) implies that $\xi = 0$ and $\eta = 0$, which does not satisfy (2.13b). Therefore, the polynomial $P(\xi, \eta)$ does not have any real roots. Consequently, its inverse is locally integrable on \mathbb{R}^2 , $P^{-1}(\xi, \eta) \in L_1^{loc}(\mathbb{R}^2)$, and, being also bounded at infinity, defines a regular distribution in $\mathcal{S}'(\mathbb{R}^2)$. This distribution $P^{-1}(\xi, \eta) \in \mathcal{S}'(\mathbb{R}^2)$ solves equation (2.11), and the fundamental solution $\mathcal{E} \in \mathcal{S}'(\mathbb{R}^2)$ of \mathbf{L} is then given by $\mathcal{E} = F^{-1}[P^{-1}(\xi, \eta)]$. Finally, the solution u of equation (2.9) can be obtained as a convolution $u = \mathcal{E} * f \equiv F^{-1}[P^{-1}(\xi, \eta)F[f]]$, which always exists in $\mathcal{D}'(\mathbb{R}^2)$ as f is compactly supported.

The second case that we consider is similar to the one discussed in Proposition 2.3. Assume that $\sigma_y = 0$, i.e., $s_y \equiv 1$. Analysis of the system (2.13) then yields that the symbol $P(\xi, \eta)$ of (2.12) has two real zeros: $(\xi, \eta) = (0, \pm\omega)$. We will study the behavior of $P(\xi, \eta)$ in the neighborhood of one of these roots. The analysis for the second root is the same.

The change of variable $\tilde{\eta} = \eta - \omega$ yields:

$$P(\xi, \tilde{\eta}) = -\frac{i\omega}{\sigma_x + i\omega} \xi^2 - \frac{\sigma_x + i\omega}{i\omega} \tilde{\eta}^2 + 2\tilde{\eta}(\omega - i\sigma_x),$$

and

$$\Re P = 2\omega\tilde{\eta} - \tilde{\eta}^2 - \frac{\omega^2}{\sigma_x^2 + \omega^2} \xi^2 = 2\omega \left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} - \tilde{\xi}^2 \right),$$

$$\Im P = -2\sigma_x\tilde{\eta} + \frac{\sigma_x}{\omega} \tilde{\eta}^2 - \frac{\sigma_x \omega}{\sigma_x^2 + \omega^2} \xi^2 = -2\sigma_x \left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} + \tilde{\xi}^2 \right),$$

where we have introduced another new variable $\tilde{\xi}^2 = \frac{\omega}{2(\sigma_x^2 + \omega^2)} \xi^2$.

In fact, we need to study the integrability of $\left| P^{-1}(\tilde{\xi}, \tilde{\eta}) \right|$ near $(\tilde{\xi}, \tilde{\eta}) = 0$. From the previous equalities we derive

$$\left| P^2(\tilde{\xi}, \tilde{\eta}) \right| = \left[\left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right)^2 + \tilde{\xi}^4 \right] (4\omega^2 + 4\sigma_x^2) + 8(\sigma_x^2 - \omega^2) \left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right) \xi^2. \quad (2.14)$$

For the second term on the right-hand side of (2.14) we obtain

$$\left| 8(\sigma_x^2 - \omega^2) \left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right) \xi^2 \right| \leq 4|\sigma_x^2 - \omega^2| \left[\left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right)^2 + \tilde{\xi}^4 \right].$$

Therefore,

$$\left| P^2(\tilde{\xi}, \tilde{\eta}) \right| \geq 8\omega^2 \left[\left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right)^2 + \tilde{\xi}^4 \right], \quad \text{for } \sigma_x^2 \geq \omega^2,$$

and

$$\left| P^2(\tilde{\xi}, \tilde{\eta}) \right| \geq 8\sigma_x^2 \left[\left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right)^2 + \tilde{\xi}^4 \right], \quad \text{for } 0 < \sigma_x^2 < \omega^2.$$

It then follows that

$$\left| P^{-1}(\tilde{\xi}, \tilde{\eta}) \right| = \left| P(\tilde{\xi}, \tilde{\eta}) \right|^{-1} \leq \mathbf{const} \left[\left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right)^2 + \tilde{\xi}^4 \right]^{-1/2}. \quad (2.15)$$

Clearly, near $\tilde{\eta} = 0$ we have $\left(\tilde{\eta} - \frac{\tilde{\eta}^2}{2\omega} \right)^2 = O(\tilde{\eta}^2)$ and therefore, the study of integrability of $\left| P^{-1}(\tilde{\xi}, \tilde{\eta}) \right|$ near $(\tilde{\xi}, \tilde{\eta}) = 0$ is reduced to determining whether or not the following integral

$$\int_{(\tilde{\xi}, \tilde{\eta}) \in U_0} \frac{d\tilde{\xi}d\tilde{\eta}}{\sqrt{\tilde{\eta}^2 + \tilde{\xi}^4}}$$

is finite for a given small neighborhood U_0 of $(\tilde{\xi}, \tilde{\eta}) = 0$. Because of the symmetry, we can analyze this integral for one quarter only, say $U_0^+ = U_0 \cap \left\{ \tilde{\xi} \geq 0, \tilde{\eta} \geq 0 \right\}$. Introducing the new variable $\tilde{\zeta}^2 = \tilde{\xi}^4$ and then polar coordinates $\tilde{\zeta} = \rho \cos \theta$, $\tilde{\eta} = \rho \sin \theta$, we obtain

$$\int_{U_0^+} \frac{d\tilde{\xi}d\tilde{\eta}}{\sqrt{\tilde{\eta}^2 + \tilde{\xi}^4}} = \int_{U_0^+} \frac{d\tilde{\zeta}d\tilde{\eta}}{2\sqrt{\tilde{\zeta}}\sqrt{\tilde{\eta}^2 + \tilde{\zeta}^2}} \leq \int_0^{\pi/2} \int_0^{\rho_0} \frac{d\rho d\theta}{2\sqrt{\rho} \cos \theta}. \quad (2.16)$$

The last integral in (2.16) is finite, and therefore we conclude that $\left| P^{-1}(\xi, \eta) \right|$ is locally absolutely integrable near $(\xi, \eta) = (0, \omega)$. A similar argument yields that $\left| P^{-1}(\xi, \eta) \right|$ is locally absolutely integrable near $(\xi, \eta) = (0, -\omega)$. Consequently, $P^{-1}(\xi, \eta) \in L_1^{loc}(\mathbb{R}^2)$. Therefore, for the case $\sigma_y = 0$, as well as for the previous case $\sigma_x \neq 0$, $\sigma_y \neq 0$, the inverse symbol $P^{-1}(\xi, \eta)$ defines a regular tempered distribution from $\mathcal{S}'(\mathbb{R}^2)$. As before, the inverse Fourier transform of $P^{-1}(\xi, \eta)$ is a fundamental solution \mathcal{E} of \mathbf{L} and the solution of (2.9) in $\mathcal{D}'(\mathbb{R}^2)$ can be constructed as $u = \mathcal{E} * f \equiv F^{-1}[P^{-1}(\xi, \eta)F[f]]$. \square

REMARK 2.6. *Theorem 2.5 guarantees the existence of the solution $u \in \mathcal{D}'(\mathbb{R}^2)$ for any right-hand side $f \in \mathcal{D}'(\mathbb{R}^2)$ such that the convolution $\mathcal{E} * f$ exists in $\mathcal{D}'(\mathbb{R}^2)$.*

For example, if we introduce the polar radius $\varrho = \sqrt{\xi^2 + \eta^2}$ in the space of dual variables (ξ, η) and require that $|F[f]| \leq \mathbf{const}(1 + \varrho)^{-\epsilon}$, $\epsilon > 0$, then obviously the convolution $\mathcal{E} * f$ exists in $\mathcal{D}'(\mathbb{R}^2)$ because $\mathcal{E} * f = F^{-1}[P^{-1}F[f]]$, $|P^{-1}(\xi, \eta)| \leq \mathbf{const}(1 + \varrho)^{-2}$, and consequently $P^{-1}F[f] \in L_1(\mathbb{R}^2)$.

REMARK 2.7. *The solution u of equation (2.9) guaranteed by Theorem 2.5 and Remark 2.6 is unique in the class of distributions u from $\mathcal{D}'(\mathbb{R}^2)$, for which the convolution with \mathcal{E} exists.*

Indeed, if $\mathbf{L}v = 0$ then $v = v * \delta = v * \mathbf{L}\mathcal{E} = \mathbf{L}v * \mathcal{E} = 0$.

PROPOSITION 2.8. *For every right-hand side $f: F[f](1 + \varrho)^{-2} \in L_1(\mathbb{R}^2)$, there is a continuous solution u of equation (2.9) that vanishes at infinity.*

Proof. As shown when proving Theorem 2.5, the inverse symbol $P^{-1}(\xi, \eta)$ of the operator \mathbf{L} is locally absolutely integrable on \mathbb{R}^2 : $P^{-1}(\xi, \eta) \in L_1^{loc}(\mathbb{R}^2)$. Also, $|P^{-1}(\xi, \eta)| \leq \mathbf{const}(1 + \varrho)^{-2}$. Therefore,

$F[f]P^{-1}(\xi, \eta) \in L_1(\mathbb{R}^2)$ and consequently, $u = \mathcal{E} * f = F^{-1}[P^{-1}F[f]]$ is continuous on \mathbb{R}^2 and $u = o(1)$, as $r \rightarrow \infty$. \square

PROPOSITION 2.9. *There exists no more than one solution $u \in \mathcal{S}'(\mathbb{R}^2)$ of equation (2.9) that vanishes at infinity.*

Proof. It is sufficient to show that the only solution in $\mathcal{S}'(\mathbb{R}^2)$ of the corresponding homogeneous equation (1.4) that vanishes at infinity is trivial. Applying the Fourier transform F to both sides of equation (1.4) we obtain $P(\xi, \eta)F[u] = 0$. For the case $\sigma_x \neq 0, \sigma_y \neq 0$, this immediately yields $F[u] \equiv 0$ and consequently, $u \equiv 0$. For the case $\sigma_x \neq 0, \sigma_y = 0$, the Fourier transform $F[u]$ may be a compactly supported distribution concentrated at two points: $(\xi, \eta) = (0, \omega)$ and $(\xi, \eta) = (0, -\omega)$. Distributions from $\mathcal{S}'(\mathbb{R}^2)$ with point-wise support are known to be linear combinations of δ -functions and their derivatives which, in turn, means that $u = F^{-1}[F[u]]$ can only be a polynomial. The boundary condition at infinity then again implies that $u \equiv 0$. \square

For the case of a non-degenerate symbol $P(\xi, \eta) \neq 0$, i.e., $\sigma_x \neq 0, \sigma_y \neq 0$, we can obtain a somewhat stronger result. In this case, $P^{-1}(\xi, \eta)$ is infinitely differentiable and therefore, the fundamental solution $\mathcal{E} = F^{-1}[P^{-1}]$ of the operator \mathbf{L} decays at infinity at least faster than any power of ϱ^{-1} . Then, one can show that the convolution with \mathcal{E} exists for at least all those functions $u \in \mathcal{D}'(\mathbb{R}^2)$ that grow at infinity slower than an exponential function. This, in particular, implies that the solution guaranteed by Proposition 2.8 is unique in the class of functions growing slower than an exponential function.

Note, general results on solvability and uniqueness for hypoelliptic equations with non-degenerate symbols in the classes of functions that grow at infinity slower than an exponent are established in [13, 14]. For the specific operator \mathbf{L} of (1.4), the hypoellipticity can be demonstrated, in particular, if $|\sigma_x - \sigma_y| < \omega$.

We, however, should mention that for the symbol $P(\xi, \eta)$ that does have real zeros ($\sigma_x \neq 0, \sigma_y = 0$), uniqueness in the class of functions that grow slower than an exponent cannot, generally speaking, be guaranteed. As can be verified by the direct differentiation, the closed form of the fundamental solution in this case is $\mathcal{E} = H_0^{(2)}(\omega \sqrt{s_x^2 x^2 + y^2})$. This function is not absolutely integrable near infinity, therefore $\mathcal{E} \notin L_1(\mathbb{R}^2)$, and consequently, the direct estimation cannot guarantee that the convolution with \mathcal{E} exists even for any bounded function on \mathbb{R}^2 .

2.3. Interface Conditions. Henceforth, we will discuss problems that contain both the areas of vacuum and PML. As has been mentioned, these formulations require special boundary conditions to be set at the interfaces, i.e., lines at which the coefficients of equation (1.4) have discontinuities. As has also been mentioned, typical geometries, for which the PML model that we are studying is implemented, are rectangular. Therefore, we will further assume that the interfaces are always straight lines aligned with the Cartesian directions.

One boundary condition at the interface is obvious — the continuity of the solution u itself. For the geometric configurations outlined above, the second boundary condition at the interface can be obtained by the following argument. Assume that the interface is the line $x = 0$, see Figure 2.1. Integrate equation (1.4) over the small rectangle $ABCD$ of width δ and height ε :

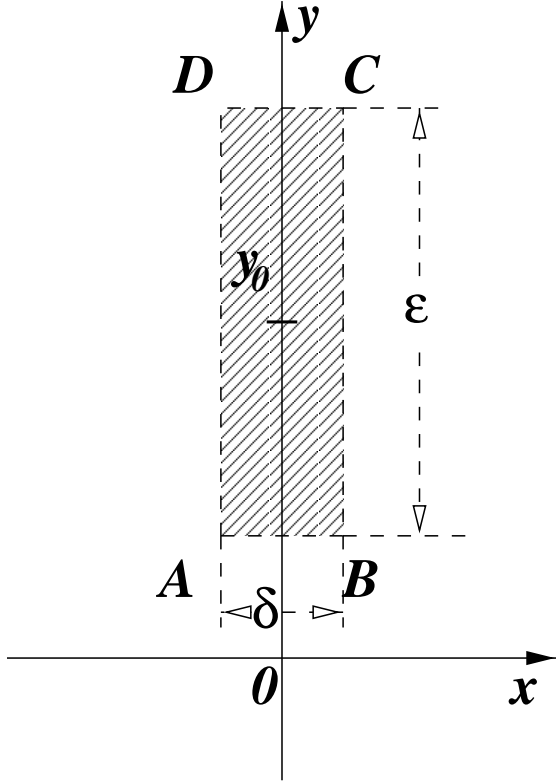


FIG. 2.1. To the derivation of the interface conditions.

$$\int_{ABCD} \left[\frac{\partial}{\partial x} \left(\frac{s_y}{s_x} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{s_x}{s_y} \frac{\partial u}{\partial y} \right) + s_x s_y \omega^2 u \right] dx dy =$$

$$\begin{aligned}
&= \int_B^C \frac{s_y}{s_x} \frac{\partial u}{\partial x} dy - \int_A^D \frac{s_y}{s_x} \frac{\partial u}{\partial x} dy + \\
&+ \int_D^C \frac{s_x}{s_y} \frac{\partial u}{\partial y} dx - \int_A^B \frac{s_x}{s_y} \frac{\partial u}{\partial y} dx + \int_{ABCD} s_x s_y \omega^2 u \, dx dy = 0
\end{aligned}$$

Let's now shrink the x -size of $ABCD$, i.e., $\delta \rightarrow 0$. The previous equality then reduces to

$$\int_{y_0 - \varepsilon/2}^{y_0 + \varepsilon/2} \left(\frac{s_y}{s_x} \frac{\partial u}{\partial x} \Big|_{x=+0} - \frac{s_y}{s_x} \frac{\partial u}{\partial x} \Big|_{x=-0} \right) dy = 0. \quad (2.17)$$

If the integrand in equation (2.17) at $y = y_0$ is equal to zero, then we have the continuity of the normal flux $\frac{s_y}{s_x} \frac{\partial u}{\partial x} \Big|_{x=+0} = \frac{s_y}{s_x} \frac{\partial u}{\partial x} \Big|_{x=-0}$, and this condition holds along the entire interface $x = 0$ as y_0 is arbitrary. If, however, we assume that the integrand in equation (2.17) at $y = y_0$ is not equal to zero, then we can always choose ε sufficiently small so that neither the real nor imaginary part of this integrand changes sign on the interval $[y_0 - \varepsilon/2, y_0 + \varepsilon/2]$ and thus immediately arrive at a contradiction. Therefore, we conclude that boundary conditions at a vertical interface $x = x_{\text{int}}$ (conditions of the continuity of solution and its normal flux) can be written as

$$u \Big|_{x_{\text{int}}-0} = u \Big|_{x_{\text{int}}+0} \quad (2.18a)$$

$$\frac{s_y}{s_x} \frac{\partial u}{\partial x} \Big|_{x_{\text{int}}-0} = \frac{s_y}{s_x} \frac{\partial u}{\partial x} \Big|_{x_{\text{int}}+0}$$

A similar argument yields boundary conditions on a horizontal interface $y = y_{\text{int}}$ in the form

$$u \Big|_{y_{\text{int}}-0} = u \Big|_{y_{\text{int}}+0} \quad (2.18b)$$

$$\frac{s_x}{s_y} \frac{\partial u}{\partial y} \Big|_{y_{\text{int}}-0} = \frac{s_x}{s_y} \frac{\partial u}{\partial y} \Big|_{y_{\text{int}}+0}$$

If, in particular, we have vacuum (1.5) to the left of the vertical interface $x = x_{\text{int}}$ and PML (1.4) with $s_y \equiv 1$ to the right of this interface, then (2.18a) reduces to

$$\begin{aligned}
u \Big|_{x=x_{\text{int}}-0} &= u \Big|_{x=x_{\text{int}}+0} \\
\frac{\partial u}{\partial x} \Big|_{x=x_{\text{int}}-0} &= \frac{1}{s_x} \frac{\partial u}{\partial x} \Big|_{x=x_{\text{int}}+0}
\end{aligned} \quad (2.19)$$

Interface conditions (2.19) will be used in the ensuing analysis, see Section 2.5.

2.4. One-Dimensional Case. To illustrate what actually happens when we have an interface between vacuum and PML in our model, we first consider the PML equation with constant coefficients in one dimension. Then (1.4) becomes

$$\mathbf{L}u \equiv \frac{\partial^2 u}{\partial x^2} + s_x^2 \omega^2 u = 0, \quad (2.20a)$$

where

$$s_x = 1 + \frac{\sigma_x}{i\omega}. \quad (2.20b)$$

We consider this equation in the interval $0 \leq x \leq L$ with the boundary condition at the outer edge of the PML given by

$$\frac{\partial u}{\partial x} + \alpha u = 0 \quad \text{for } x = L. \quad (2.21)$$

For $x < 0$ we assume that we have the Helmholtz equation. Therefore, the general solution in the PML layer is given by

$$u = Ae^{i\omega s_x x} + Be^{-i\omega s_x x} = Ae^{\sigma+i\omega x} + Be^{-(\sigma+i\omega)x}. \quad (2.22)$$

The solution for the outgoing wave is $A = 0$. Substituting (2.22) into (2.21) we find that

$$\frac{A}{B} = -\frac{\alpha - \sigma - i\omega}{\alpha + \sigma + i\omega} e^{-2(\sigma+i\omega)L} \quad (2.23)$$

or

$$\left| \frac{A}{B} \right| = \left| \frac{\alpha - \sigma - i\omega}{\alpha + \sigma + i\omega} \right| e^{-2\sigma L}. \quad (2.24)$$

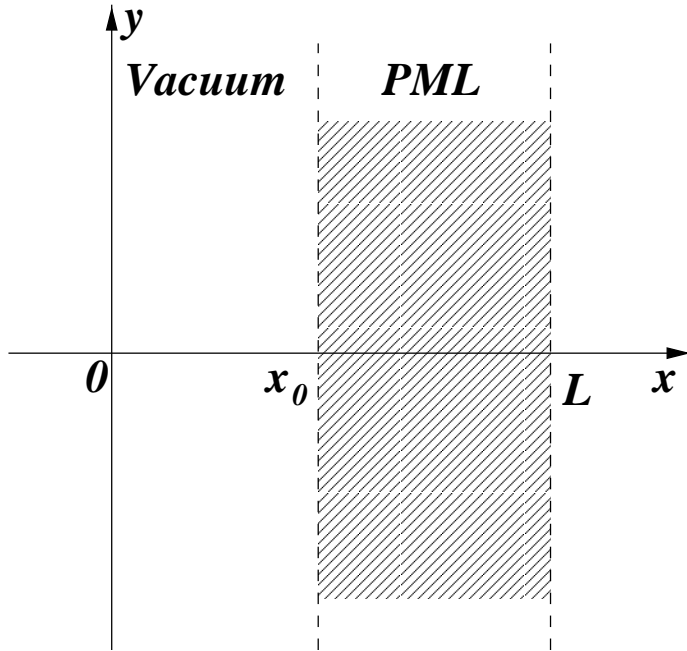


FIG. 2.2. Schematic geometric setup for the y -aligned PML on the entire plane.

have a vacuum medium governed by the Helmholtz equation $\Delta u + \omega^2 u = f$. The sources f that drive the solution are assumed to be compactly supported with $\text{supp} f \subset \{(x, y) | x \leq x_0\}$. To the right of the interface $x = x_0$ we have a medium governed by the homogeneous PML equation (1.4) with $\sigma_x \neq 0$ and $\sigma_y = 0$, i.e., s_x complex and $s_y \equiv 1$. The PML is terminated at the location $x = L$, $L > x_0$. In this case we require that $u|_{x=L} = 0$; the homogeneous Dirichlet boundary condition is chosen mostly for the reason of simplicity of the analysis, other boundary conditions for termination of the PML can be used, e.g., (2.21). In particular, the PML may stretch all the way to infinity (this formally means letting $L = +\infty$), in this case we require that the solution be bounded at infinity, i.e., $|u| < \infty$ as $x \rightarrow +\infty$.

Note that if $\sigma = 0$ and $\alpha = i\omega$ then $A = 0$, i.e., we get the exact solution even though the Sommerfeld radiation is imposed at a finite location. (Condition (2.21) transforms into the Sommerfeld radiation condition if $\alpha = i\omega$.) However, this “miracle” only occurs in one dimension. If α is real, formula (2.24) becomes

$$\left| \frac{A}{B} \right| = \sqrt{\frac{(\alpha - \sigma)^2 + \omega^2}{(\alpha + \sigma)^2 + \omega^2}} e^{-2\sigma L} \quad (2.25)$$

Thus, A approaches zero exponentially fast as $L \rightarrow \infty$. For both the Dirichlet and Neumann boundary conditions ($\alpha = 0$ and $\alpha = \infty$, respectively) the coefficient in front of the exponential decay is one. To minimize this coefficient we would choose $\alpha = \sigma$.

2.5. Combined Problem on the Entire Plane. The simplest two-dimensional problem formulation that involves both the domains of vacuum and PML is shown schematically in Figure 2.2. We assume that to the left of the vertical interface $x = x_0$ we

We will use the subscript “ v ” to denote the solution u_v in the vacuum area $x < x_0$ and subscript “ p ” to denote the PML solution u_p for $x > x_0$. We now apply the Fourier transform in the y -direction:

$$\hat{u} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u e^{-iky} dy,$$

\hat{u} is a function of the variable x and parameter (wavenumber) k . As the governing equation in the vacuum area is assumed homogeneous near the interface, then (1.5) is transformed into the following family of ODEs parameterized by the continuous wavenumber k :

$$\hat{u}_v'' + (\omega^2 - k^2)\hat{u}_v = 0, \quad -\infty < k < \infty, \quad (2.26a)$$

where double prime denotes the second derivative with respect to x and \hat{u}_v stands for $\hat{u}_v(x, k)$. Similarly, in the PML region we obtain:

$$\hat{u}_p'' + s_x^2(\omega^2 - k^2)\hat{u}_p = 0, \quad -\infty < k < \infty, \quad (2.26b)$$

where again $\hat{u}_p = \hat{u}_p(x, k)$.

We will now discuss the behavior of the solution u_v at $x = x_0$ caused by the adjacent PML. If we were solving the original Helmholtz equation on the semi-plane $x \leq x_0$ and requiring that the semi-plane solution coincide with the corresponding fragment of the solution on the entire plane driven by the same sources and satisfying the Sommerfeld conditions at infinity then we would have had to impose some artificial boundary conditions (ABCs), see [17], at $x = x_0$. The sole purpose of the ABCs is to guarantee the desirable “far-field” behavior of the solution once it is actually calculated only on a portion of the original domain, i.e., on the subdomain obtained by truncation. In the specific case that we are studying, the truncated subdomain is the left semi-plane $x \leq x_0$ and the desirable far-field behavior of the solution near infinity that corresponds to boundary conditions (2.6) is that this solution should be composed of outgoing waves only. It is also known that the decay of the solution at infinity prescribed by (2.6a) is a consequence of the Sommerfeld radiation condition (2.6b).

The key idea behind the construction of ABCs (see [17]) is that the boundary conditions should enforce the proper mode selection that corresponds to the desirable far-field behavior of the solution. Namely, for each k equation (2.26a) has two eigensolutions. If $\omega^2 > k^2$ these eigensolutions are

$$\hat{u}_v^{(1)} = \exp\left(i\sqrt{\omega^2 - k^2}x\right) \quad (2.27a)$$

and

$$\hat{u}_v^{(2)} = \exp\left(-i\sqrt{\omega^2 - k^2}x\right). \quad (2.27b)$$

If $\omega^2 < k^2$ the eigensolutions are

$$\hat{u}_v^{(1)} = \exp\left(\sqrt{k^2 - \omega^2}x\right) \quad (2.28a)$$

and

$$\hat{u}_v^{(2)} = \exp\left(-\sqrt{k^2 - \omega^2}x\right). \quad (2.28b)$$

Solutions (2.27) correspond to the traveling waves; according to the desirable “outgoing” far-field behavior we need to select the right-traveling mode $\hat{u}_v^{(2)}$ of (2.27b) (see [17]). Solutions (2.28) correspond to the evanescent waves, to ensure the boundedness of the solution at infinity it is sufficient to select the decaying mode $\hat{u}_v^{(2)}$ of (2.28b). In both cases, the selection can actually be enforced by specifying similar first-order boundary conditions (in the y -Fourier space) at $x = x_0$:

$$\left. \frac{d\hat{u}_v}{dx} + i\sqrt{\omega^2 - k^2}\hat{u}_v \right|_{x=x_0-0} = 0, \quad \text{for } \omega^2 > k^2, \quad (2.29a)$$

$$\left. \frac{d\hat{u}_v}{dx} + \sqrt{k^2 - \omega^2}\hat{u}_v \right|_{x=x_0-0} = 0, \quad \text{for } \omega^2 < k^2. \quad (2.29b)$$

It is straightforward that the mode $\hat{u}_v^{(2)}$ of (2.27b) turns (2.29a) into an identity, whereas the mode $\hat{u}_v^{(1)}$ of (2.27a) does not satisfy (2.29a). Similarly, the mode $\hat{u}_v^{(2)}$ of (2.28b) satisfies (2.29b) identically but the mode $\hat{u}_v^{(1)}$ of (2.28a) does not satisfy (2.29b). We note that boundary conditions (2.29) can also be obtained by an analysis of the Wronskians, see [17]. The degenerate intermediate case $\omega^2 - k^2 = 0$ will be analyzed at the end of the section.

The eigenmodes of equations (2.26b) are

$$\hat{u}_p^{(1)} = \exp\left(i s_x \sqrt{\omega^2 - k^2} x\right) \quad (2.30a)$$

and

$$\hat{u}_p^{(2)} = \exp\left(-i s_x \sqrt{\omega^2 - k^2} x\right) \quad (2.30b)$$

for $\omega^2 > k^2$ and

$$\hat{u}_p^{(1)} = \exp\left(s_x \sqrt{k^2 - \omega^2} x\right) \quad (2.31a)$$

and

$$\hat{u}_p^{(2)} = \exp\left(-s_x \sqrt{k^2 - \omega^2} x\right) \quad (2.31b)$$

for $\omega^2 < k^2$.

We first assume that the PML has infinite thickness, i.e., $L = +\infty$, see Figure 2.2. Substituting the expression for s_x from (1.3) into (2.30) and (2.31), we easily see that the modes $\hat{u}_p^{(2)}$ of (2.30b) and (2.31b) vanish as $x \rightarrow +\infty$, whereas the modes $\hat{u}_p^{(1)}$ of (2.30a) and (2.31a) grow without bound. To ensure that the PML solution be bounded at infinity, we select only decaying modes and thus arrive at the following family of boundary conditions

$$\left. \frac{d\hat{u}_p}{dx} + i s_x \sqrt{\omega^2 - k^2} \hat{u}_p \right|_{x=x_0+0} = 0, \quad \text{for } \omega^2 > k^2, \quad (2.32a)$$

$$\left. \frac{d\hat{u}_p}{dx} + s_x \sqrt{k^2 - \omega^2} \hat{u}_p \right|_{x=x_0+0} = 0, \quad \text{for } \omega^2 < k^2. \quad (2.32b)$$

We now use interface conditions (2.19) for $x_{\text{int}} = x_0$ and immediately conclude that boundary conditions (2.32) that follow from the requirement of boundedness at infinity, together with (2.19) imply (2.29). In other words, an infinitely thick PML, in which the solution is bounded at infinity, adjacent to an area of vacuum implies the same behavior of the solution at the straight interface as would have been displayed by the solution to the vacuum problem if solved on the entire plane with the additional requirement of wave radiation in the far field.

We therefore conclude that the PML can basically “relax” the boundary conditions at infinity in the sense that we can require only boundedness instead of the additional radiation conditions. On the other hand, from the standpoint of numerical implementation an infinitely thick PML still does not provide for a

formulation that can be immediately discretized and solved on the computer. Instead, we now consider a PML with a finite thickness.

For every Fourier mode k , the general solution \hat{u}_p in the PML can be written as

$$\hat{u}_p(x, k) = C_1 \hat{u}_p^{(1)}(x, k) + C_2 \hat{u}_p^{(2)}(x, k),$$

where C_1 and C_2 are arbitrary constants (different for different k). As the PML is now terminated at a finite location $x = L$ with the homogeneous Dirichlet boundary condition, we obtain

$$C_1 \hat{u}_p^{(1)}(L, k) + C_2 \hat{u}_p^{(2)}(L, k) = 0,$$

and consequently

$$C_1 = -C_2 \exp\left(-2is_x \sqrt{\omega^2 - k^2} L\right), \quad \text{for } \omega^2 > k^2, \quad (2.33a)$$

$$C_1 = -C_2 \exp\left(-2s_x \sqrt{k^2 - \omega^2} L\right), \quad \text{for } \omega^2 < k^2. \quad (2.33b)$$

The corresponding vacuum solution for the mode k is given by

$$\hat{u}_v(x, k) = A_1 \hat{u}_v^{(1)}(x, k) + A_2 \hat{u}_v^{(2)}(x, k),$$

A_1 and A_2 are constants. Using interface conditions (2.19) at $x_{\text{int}} = x_0$ for $\omega^2 > k^2$, we arrive at

$$\begin{aligned} & A_1 \exp(i\sqrt{\omega^2 - k^2} x_0) + A_2 \exp(-i\sqrt{\omega^2 - k^2} x_0) = \\ & = C_1 \exp(is_x \sqrt{\omega^2 - k^2} x_0) + C_2 \exp(-is_x \sqrt{\omega^2 - k^2} x_0), \\ & i\sqrt{\omega^2 - k^2} A_1 \exp(i\sqrt{\omega^2 - k^2} x_0) - i\sqrt{\omega^2 - k^2} A_2 \exp(-i\sqrt{\omega^2 - k^2} x_0) = \\ & = \frac{1}{s_x} \left[is_x \sqrt{\omega^2 - k^2} C_1 \exp(is_x \sqrt{\omega^2 - k^2} x_0) - is_x \sqrt{\omega^2 - k^2} C_2 \exp(-is_x \sqrt{\omega^2 - k^2} x_0) \right], \end{aligned}$$

which, together with (2.33a), yields

$$\begin{aligned} A_1 \exp(i\sqrt{\omega^2 - k^2} x_0) &= C_1 \exp(is_x \sqrt{\omega^2 - k^2} x_0) \\ A_2 \exp(-i\sqrt{\omega^2 - k^2} x_0) &= C_2 \exp(-is_x \sqrt{\omega^2 - k^2} x_0) \end{aligned} \quad (2.34a)$$

and consequently

$$\begin{aligned} \frac{A_1}{A_2} &= \frac{C_1}{C_2} \exp\left(2i(s_x - 1)\sqrt{\omega^2 - k^2} x_0\right) = \\ &= -\exp\left(-2i\sqrt{\omega^2 - k^2} L\right) \exp\left(-2\sqrt{1 - k^2/\omega^2} s_x (L - x_0)\right). \end{aligned} \quad (2.34b)$$

Similarly, for $\omega^2 < k^2$ using (2.33b) we obtain

$$\begin{aligned} A_1 \exp(\sqrt{k^2 - \omega^2} x_0) &= C_1 \exp(s_x \sqrt{k^2 - \omega^2} x_0) \\ A_2 \exp(-\sqrt{k^2 - \omega^2} x_0) &= C_2 \exp(-s_x \sqrt{k^2 - \omega^2} x_0) \end{aligned} \quad (2.34c)$$

and consequently

$$\begin{aligned} \frac{A_1}{A_2} &= \frac{C_1}{C_2} \exp\left(2(s_x - 1)\sqrt{k^2 - \omega^2}x_0\right) = \\ &= -\exp\left(-2\sqrt{k^2 - \omega^2}L\right) \exp\left(2i\sqrt{k^2/\omega^2 - 1}\sigma_x(L - x_0)\right). \end{aligned} \quad (2.34d)$$

With the help of relations (2.34), (2.29) and (2.32), we will now construct the one-dimensional fundamental solutions. First, denoting

$$\hat{\mathcal{E}}_0(x, k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{E}_0(x, y) e^{-iky} dy = \frac{1}{\sqrt{2\pi}} \frac{\pi}{2i} \int_{-\infty}^{\infty} H_0^{(2)}\left(\omega\sqrt{x^2 + y^2}\right) e^{-iky} dy$$

(see (2.8)), and Fourier transforming equation (2.7) with respect to y , we conclude that for each k the function $\hat{\mathcal{E}}_0(x, k)$ satisfies

$$\hat{\mathcal{E}}_0'' + (\omega^2 - k^2)\hat{\mathcal{E}}_0 = \delta(x). \quad (2.35)$$

The solution to equation (2.35) has to be symmetric with respect to the origin (the two-dimensional fundamental solution \mathcal{E}_0 of (2.8) is symmetric) and composed of a right traveling/decaying wave as $x \geq 0$ and left traveling/decaying wave as $x \leq 0$. This solution is unique and given by

$$\hat{\mathcal{E}}_0(x, k) = -\frac{1}{2i\sqrt{\omega^2 - k^2}} \exp\left(-i\sqrt{\omega^2 - k^2}|x|\right) \quad \text{for } \omega^2 > k^2 \quad (2.36a)$$

and

$$\hat{\mathcal{E}}_0(x, k) = -\frac{1}{2\sqrt{k^2 - \omega^2}} \exp\left(-\sqrt{k^2 - \omega^2}|x|\right) \quad \text{for } \omega^2 < k^2. \quad (2.36b)$$

For the case of an infinitely thick PML, $L = +\infty$, see Figure 2.2, we have instead of (2.35):

$$\begin{aligned} \hat{\mathcal{E}}_{0v}'' + (\omega^2 - k^2)\hat{\mathcal{E}}_{0v} &= \delta(x), \quad x \leq x_0, \\ \hat{\mathcal{E}}_{0p}'' + s_x^2(\omega^2 - k^2)\hat{\mathcal{E}}_{0p} &= 0, \quad x \geq x_0, \end{aligned} \quad (2.37)$$

with the interface conditions (2.19) for $x = x_0$. For equations (2.37), we still require that the left branch of the solution, i.e., $\hat{\mathcal{E}}_{0v}$ for $x \leq 0$, be a left traveling wave (for $\omega^2 > k^2$) or left decaying evanescent wave (for $\omega^2 < k^2$); however, for $x \geq 0$, more precisely, $x \rightarrow +\infty$, we require only boundedness of $\hat{\mathcal{E}}_{0p}$. This boundedness, interpreted as boundary conditions (2.32) and transformed into (2.29) with the help of (2.19), implies that $\hat{\mathcal{E}}_{0v}$ of (2.37) coincides with $\hat{\mathcal{E}}_0$ of (2.35), (2.36) for $x \leq x_0$.

Let us now consider the PML of a finite thickness, see Figure 2.2. We will use notation \mathcal{E} for the corresponding fundamental solution although it is different from \mathcal{E} of Section 2.2 as there we discussed the fundamental solution for the entire plane filled with PML. Equations that we are solving to find the one-dimensional fundamental solution $\hat{\mathcal{E}} = \hat{\mathcal{E}}(x, k)$ look similar to (2.37):

$$\begin{aligned} \hat{\mathcal{E}}_v'' + (\omega^2 - k^2)\hat{\mathcal{E}}_v &= \delta(x), \quad x \leq x_0, \\ \hat{\mathcal{E}}_p'' + s_x^2(\omega^2 - k^2)\hat{\mathcal{E}}_p &= 0, \quad x \geq x_0, \end{aligned} \quad (2.38)$$

however, the right branch of this fundamental solution, i.e., $\hat{\mathcal{E}}(x, k)$ for $x \geq 0$, is now composed of both waves and the relative weight of each component is determined by the PML thickness or in other words, prescribed by equations (2.34). Physically, the presence of the second wave (which is absent in (2.36)) can

be interpreted as “reflection,” this “reflected” wave “propagates” all the way to $x \rightarrow -\infty$ and therefore, the left branch of the fundamental solution $\hat{\mathcal{E}}$ still consists of the wave of one type only. Thus, for $\omega^2 > k^2$ we are constructing $\hat{\mathcal{E}}$ in the form

$$\hat{\mathcal{E}}(x, k) = \begin{cases} A \exp\left(i\sqrt{\omega^2 - k^2}x\right), & \text{if } x \leq 0, \\ A_1 \exp\left(i\sqrt{\omega^2 - k^2}x\right) + A_2 \exp\left(-i\sqrt{\omega^2 - k^2}x\right), & \text{if } x \geq 0, \end{cases}$$

where the relation between A_1 and A_2 is known and given by (2.34a), (2.34b). The continuity at $x = 0$ yields $A = A_1 + A_2$ and we therefore obtain

$$\hat{\mathcal{E}}(x, k) = \begin{cases} -\frac{1 + A_1/A_2}{2i\sqrt{\omega^2 - k^2}} \exp\left(i\sqrt{\omega^2 - k^2}x\right), & \text{if } x \leq 0, \\ -\frac{A_1/A_2}{2i\sqrt{\omega^2 - k^2}} \exp\left(i\sqrt{\omega^2 - k^2}x\right) - \frac{1}{2i\sqrt{\omega^2 - k^2}} \exp\left(-i\sqrt{\omega^2 - k^2}x\right), & \text{if } x \geq 0. \end{cases} \quad (2.39a)$$

Similarly, for $\omega^2 < k^2$ we have

$$\hat{\mathcal{E}}(x, k) = \begin{cases} -\frac{1 + A_1/A_2}{2\sqrt{k^2 - \omega^2}} \exp\left(\sqrt{k^2 - \omega^2}x\right), & \text{if } x \leq 0, \\ -\frac{A_1/A_2}{2\sqrt{k^2 - \omega^2}} \exp\left(\sqrt{k^2 - \omega^2}x\right) - \frac{1}{2\sqrt{k^2 - \omega^2}} \exp\left(-\sqrt{k^2 - \omega^2}x\right), & \text{if } x \geq 0. \end{cases} \quad (2.39b)$$

Then, substituting A_1/A_2 from (2.34b) and (2.34d), we obtain that the reflected wave due to the finite thickness of the PML is given by

$$\hat{\mathcal{E}}(x, k) - \hat{\mathcal{E}}_0(x, k) = \frac{1}{2i\sqrt{\omega^2 - k^2}} \exp\left(i\sqrt{\omega^2 - k^2}(x - 2L)\right) \exp\left(-2\sqrt{1 - k^2/\omega^2}\sigma_x(L - x_0)\right) \quad (2.40a)$$

for $\omega^2 > k^2$ and

$$\hat{\mathcal{E}}(x, k) - \hat{\mathcal{E}}_0(x, k) = \frac{1}{2\sqrt{k^2 - \omega^2}} \exp\left(\sqrt{k^2 - \omega^2}(x - 2L)\right) \exp\left(2i\sqrt{k^2/\omega^2 - 1}\sigma_x(L - x_0)\right) \quad (2.40b)$$

for $\omega^2 < k^2$, where in both (2.40a) and (2.40b) we always assume $x \leq x_0$. We notice that this reflected wave is continuous with its derivatives, which another time shows that the δ -source drives “directly” only the original solution $\hat{\mathcal{E}}_0$ of (2.36) and the additional contribution, i.e., reflection, is caused by the finite thickness of the PML.

From (2.40a) we conclude that the amplitude of each traveling wave in the reflected field decays exponentially as the thickness of the PML $L - x_0$ grows (as long as $\sigma_x > 0$). Reflected waves of the other family, given by expressions (2.40b), are evanescent exponentially decaying waves as $x \rightarrow -\infty$. These two facts already indicate that thicker the PML less reflection we get and as the PML thickness approaches infinity we eventually arrive at the pure reflectionless solution obtained for the case $L = +\infty$.

To estimate the magnitude of the reflection in the original rather than Fourier space, we consider a particular case: $x_0 = 0$ and $x = 0$. In other words, we consider the driving δ -source located exactly on the interface between the vacuum and PML and we also calculate the reflected field right at this interface. In this case, instead of (2.40), we have:

$$\hat{\mathcal{E}}(0, k) - \hat{\mathcal{E}}_0(0, k) = \frac{1}{2i\sqrt{\omega^2 - k^2}} \exp\left(-is_x\sqrt{\omega^2 - k^2}2L\right) \quad \text{for } \omega^2 > k^2 \quad (2.41a)$$

and

$$\hat{\mathcal{E}}(0, k) - \hat{\mathcal{E}}_0(0, k) = \frac{1}{2\sqrt{k^2 - \omega^2}} \exp\left(-s_x \sqrt{k^2 - \omega^2} 2L\right) \quad \text{for } \omega^2 < k^2. \quad (2.41b)$$

Comparing formulae (2.41) with (2.36), we see that they are almost identical except for the sign as well as $|x|$ in the exponent being replaced by $s_x \cdot 2L$. Thus, we conclude that in the original space the reflected field at $x = 0$ (for $x_0 = 0$ and $0 < L < \infty$) is given by

$$\mathcal{E}(0, y) - \mathcal{E}_0(0, y) = -\frac{\pi}{2i} H_0^{(2)}\left(\omega \sqrt{4s_x^2 L^2 + y^2}\right). \quad (2.42)$$

Denote $\tilde{q}^2 = 4s_x^2 L^2 + y^2$, $q^2 = 4L^2 + y^2$ and also $\mu = \sigma_x/\omega > 0$, $\cos\phi = 2L/q$. Then, $\tilde{q}^2 = q^2(1 - (\mu^2 + 2i\mu)\cos^2\phi)$. From this expression it is easy to see that $\Im(\tilde{q}/q) < 0$. As for large $|z|$ ($z \in \mathbb{C}$) we have $H_0^{(2)}(z) \sim (1/\sqrt{z})\exp(-iz)$, we conclude that the reflected field (2.42), which is $\sim H_0^{(2)}(\omega q(\tilde{q}/q))$, is exponentially small in L . This result is similar to that of Section 2.4 regarding the one-dimensional case.

It remains to address the degenerate case $\omega^2 = k^2$. In this case, both equations (2.26a) and (2.26b) reduce to

$$\hat{u}'' = 0. \quad (2.43)$$

We first notice, that for the version of PML that we are studying here, equation (2.43) is the same for both vacuum and PML areas. We also notice that unlike equations (2.26) considered earlier, equation (2.43) does not have a bounded fundamental solution. Indeed, an obvious symmetric solution of the equation $\hat{\mathcal{E}}_0'' = \delta(x)$ is $\hat{\mathcal{E}}_0 = |x|/2$; a constant can be added to $\hat{\mathcal{E}}_0$ for all $x \in (-\infty, +\infty)$, which still leaves it a symmetric unbounded fundamental solution. It is also known that the fundamental solution is basically determined up to an additive term that solves the pure homogeneous equation (2.43). The general solution of (2.43) is a linear combination of a constant and linear function; by adding such solutions to $\hat{\mathcal{E}}_0$ one can obtain a family of fundamental solutions that will, generally speaking, be non-symmetric but still unbounded at least in one direction (either $x \rightarrow +\infty$ or $x \rightarrow -\infty$). In particular, by adding a proper solution of the homogeneous equation, we can always achieve $\hat{\mathcal{E}}(L) = 0$, which will account for the termination of PML at $x = L$.

For problems on the entire \mathbb{R}^2 considered in this section, one uses the continuous Fourier transform for transition between the two-dimensional equation and the corresponding family of one-dimensional equations. It is clear that the values of the function at two particular points, whatever these values might be, are not going to change the value of the integral when going back to original variables, i.e., calculating the solution by means of the inverse Fourier transform (Fourier integral). In particular, the fact that the one-dimensional fundamental solution for $\omega^2 = k^2$ is unbounded is not going to affect the boundedness and even decay of the solution in original variables as $r \rightarrow \infty$. This property in a slightly different form has been demonstrated and analyzed in [15]. In other words, this means that when a problem is solved using continuous Fourier integrals, the values $k = \pm\omega$, for which there is no bounded fundamental solution, can be effectively disregarded. The situation can be entirely different when the domain in the y -direction is finite and instead of the Fourier integral one uses Fourier series; in this case the weight of each wavenumber is finite (as opposed to the continuous case when each particular k makes an infinitesimal contribution to the Fourier integral) and consequently, there might not be an overall bounded solution at all. In conclusion, we note that rigorous analysis of similar phenomena based on introduction of the so-called generalized principles of limitary absorption is contained in [11, 12].

2.6. Combined Problem in the Waveguide. We now consider a semi-infinite x -aligned waveguide that stretches from $x = 0$ to $x = +\infty$ and is π -wide in the y -direction, see Figure 2.3. We assume that the solution is equal to zero on the walls of the waveguide and bounded as $x \rightarrow +\infty$.

First, it is clear that if the entire waveguide was filled only with vacuum, then the solution to the Helmholtz equation (1.5) with Dirichlet boundary conditions on the walls of the waveguide would not, generally speaking, be unique. In other words, there will be a non-zero solution with zero Dirichlet boundary data: $u = 0$ at $x = 0$, $y = 0$, and $y = \pi$, and zero source terms. This non-zero solution can actually be

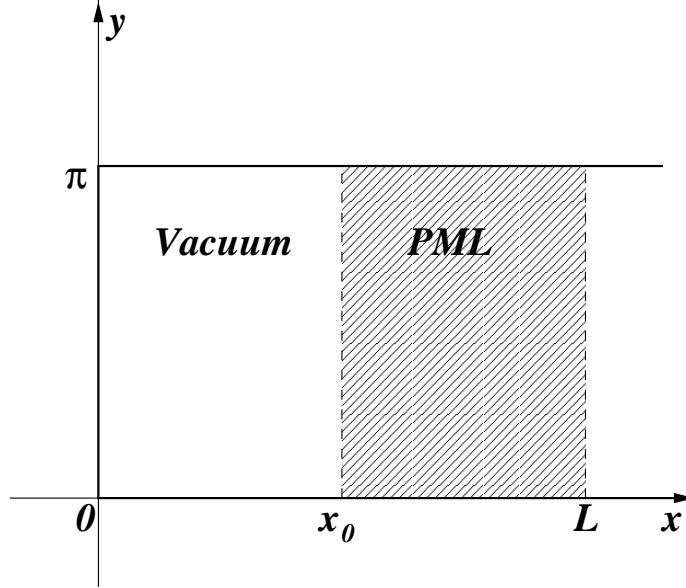


FIG. 2.3. Schematic geometric setup for the PML on the x -aligned semi-infinite waveguide.

constructed by using the sine Fourier series expansion in the transversal y -direction. Indeed, any solution $u(x, y)$ in the waveguide that turns into zero on its wall can be represented as a sum of this series for each x :

$$u(x, y) = \sum_{k=1}^{\infty} \hat{u}(x, k) \sin(ky), \quad (2.44a)$$

where

$$\hat{u}(x, k) = \frac{2}{\pi} \int_0^{\pi} u(x, y) \sin(ky) dy. \quad (2.44b)$$

Then the longitudinal x -modes $\hat{u}(x, k)$ are still given by expressions (2.27) and (2.28), the only difference is that now the spectrum is discrete rather than continuous — the wavenumbers k are integers. To construct a non-trivial solution for the zero boundary data and zero source terms, we can take any k such that $\omega^2 > k^2$ (provided that ω is sufficiently large so that there exist traveling waves in the waveguide of this particular width) and then consider the corresponding longitudinal solution in the form $\hat{u} = \hat{u}_v^{(1)} - \hat{u}_v^{(2)} = 2 \sin(\sqrt{\omega^2 - k^2}x)$; this yields the overall solution in the form $u = 2 \sin(ky) \sin(\sqrt{\omega^2 - k^2}x)$, which is obviously bounded at infinity and equal to zero at $x = 0$ and $y = 0, y = \pi$. We note, that non-uniqueness can develop only on the traveling part of the spectrum, evanescent waves (2.28) are given by real exponential function and they must all be zero to satisfy the zero Dirichlet boundary condition at $x = 0$ (because $\sin(ky)$, $k = 1, 2, \dots$, form a full orthogonal system). To guarantee uniqueness for the pure Helmholtz equation in the waveguide, we need, as before, to require that some kind of a radiation principle be met, e.g., only right-traveling waves (2.27b) be present in the solution. In this case, the zero Dirichlet boundary condition at $x = 0$ will again imply that all components are actually zero.

As opposed to the previous case, the solution for the waveguide filled entirely with the PML medium is unique. Indeed, consider a solution $u(x, y)$ of equation (1.4) with $\sigma_x \neq 0$, $\sigma_y = 0$, in the waveguide shown in Figure 2.3 with boundary conditions $u = 0$ at $x = 0$, $y = 0$, and $y = \pi$, and bounded as $x \rightarrow +\infty$. As the sine functions $\sin(ky)$, $k = 1, 2, \dots$, form a full orthogonal system in $L_2[0, \pi]$ with zero boundary conditions at 0 and π , we expand $u(x, y)$ in the sine Fourier series (2.44a) and see that for each $k = 1, 2, \dots$, the component $\hat{u}(x, k)$ satisfies equation (2.26b) for $x \in [0, +\infty)$. The condition of boundedness at infinity

implies that only the decaying longitudinal modes (2.30b) and (2.31b) can be taken. Then, the conditions $\hat{u}(0, k) = 0$, $k = 1, 2, \dots$, that follow from the zero Dirichlet boundary condition for $u(x, y)$ at $x = 0$, immediately yield that each Fourier component is equal to zero and therefore, the entire solution is zero.

Let us also note that for both preliminary formulations analyzed above, we may need to consider a special case $\omega^2 - k^2 = 0$ if ω is integer. In this case, the one-dimensional equation that needs to be solved in Fourier space is $\hat{u}'' = 0$, the two linearly independent solutions are $\hat{u}^{(1)} = \text{const}$ and $\hat{u}^{(2)} = x$, the second one is prohibited by the condition of boundedness at infinity (each term of the series has “finite weight,” as opposed to the case of the continuous Fourier transform analyzed in the previous section), the first one is prohibited by the zero Dirichlet boundary condition at $x = 0$. In the uniqueness proofs that follow, we will not be taking the case $\omega^2 = k^2$ into consideration because as we have just seen, no nontrivial solution of the homogeneous problem that we are studying can exist for this wavenumber.

We now consider the waveguide with both vacuum and PML areas and first assume that the PML is infinitely thick, i.e., $L = +\infty$, see Figure 2.3. The following theorem establishes uniqueness by showing that the homogeneous problem with zero Dirichlet boundary conditions has only trivial solution.

THEOREM 2.10. *Let the PML in the waveguide be infinitely thick, $L = +\infty$, see Figure 2.3. Let $u = u(x, y)$ satisfy equation (1.5) in the vacuum area of the waveguide, equation (1.4) with $\sigma_x \neq 0$, $\sigma_y = 0$, in the PML area, interface conditions (2.19) at $x_{\text{int}} = x_0$, be equal to zero, $u = 0$, at $x = 0$, $y = 0$, and $y = \pi$, and bounded, $|u| < \infty$, as $x \rightarrow +\infty$. Then, $u \equiv 0$.*

Proof. First, expand $u(x, y)$ for each $x \geq 0$ in the sine Fourier series (2.44a) with respect to the transversal coordinate y . Then, for each $k = 1, 2, \dots$, the component $\hat{u}(x, k)$ satisfies equation (2.26a) for $0 \leq x \leq x_0$ and equation (2.26b) for $x \geq x_0$. Boundedness at infinity implies that only the decaying longitudinal modes (2.30b) and (2.31b) are present in the solution in the PML area. Then, from the interface conditions (2.19) and relations (2.34a), (2.34c) that follow from (2.19) we conclude that only the modes (2.27b) and (2.28b) can be present in the solution in the vacuum area, i.e., $A_1(k) = 0$.

Let us now denote the complex conjugate of u by \bar{u} and apply Green’s formula to the vacuum area:

$$\int_{\text{vacuum}} [\bar{u}(\Delta u + \omega^2 u) - u(\Delta \bar{u} + \omega^2 \bar{u})] dx dy = \int_0^\pi \left[\bar{u} \frac{\partial u}{\partial x} - u \frac{\partial \bar{u}}{\partial x} \right] \Big|_{x=x_0} dy = 0. \quad (2.45)$$

Substituting the sine Fourier expansion (2.44a) for u and \bar{u} at $x = x_0$ into the second integral of (2.45), using the orthogonality of $\sin(ky)$, $k = 1, 2, \dots$, and also differentiating (2.44a) with respect to x to obtain $u'_x|_{x=x_0}$ and $\bar{u}'_x|_{x=x_0}$ for (2.45), we arrive at

$$\sum_{k=1}^{\infty} |A_2(k)|^2 \left(\bar{\hat{u}}_v^{(2)} \frac{d}{dx} \hat{u}_v^{(2)} - \hat{u}_v^{(2)} \frac{d}{dx} \bar{\hat{u}}_v^{(2)} \right) = 0. \quad (2.46)$$

From (2.28b) we see that if $\omega^2 < k^2$ then $\hat{u}_v^{(2)}(x, k) = \bar{\hat{u}}_v^{(2)}(x, k)$ and therefore, the expression in brackets in (2.46) turns into zero. Consequently, from (2.27b) and (2.46) we obtain

$$\sum_{k^2 < \omega^2} -2i\sqrt{\omega^2 - k^2} |A_2(k)|^2 = 0,$$

which means that $|A_2(k)| = 0$ for $k^2 < \omega^2$ and therefore, the waveguide solution $u = u(x, y)$ does not contain any traveling modes. Thus, if $u(x, y)$ is still nontrivial, it can be composed of the evanescent modes only.

We will now apply the methodology similar to the one used when proving Theorem 2.1. Introduce some $x_1 > x_0$ and notice that the operator \mathbf{L} of (1.4) reduces to $\Delta + \omega^2$ in the vacuum area:

$$\int_{\substack{0 \leq x \leq x_1 \\ 0 \leq y \leq \pi}} (\bar{u} \mathbf{L} u) dx dy = - \int_{\substack{0 \leq x \leq x_0 \\ 0 \leq y \leq \pi}} \left[\left| \frac{\partial u_v}{\partial x} \right|^2 + \left| \frac{\partial u_v}{\partial y} \right|^2 - \omega^2 |u_v|^2 \right] dx dy + \int_0^\pi \bar{u}_v \frac{\partial u_v}{\partial x} \Big|_{x=x_0} dy -$$

$$\begin{aligned}
& - \int_{\substack{x_0 \leq x \leq x_1 \\ 0 \leq y \leq \pi}} \left[\frac{1}{s_x} \left| \frac{\partial u_p}{\partial x} \right|^2 + s_x \left| \frac{\partial u_p}{\partial y} \right|^2 - s_x \omega^2 |u_p|^2 \right] dx dy + \int_0^\pi \frac{1}{s_x} \bar{u}_p \left(-\frac{\partial u_p}{\partial x} \right) \Big|_{x=x_0} dy + \\
& \quad + \int_0^\pi \frac{1}{s_x} \bar{u}_p \frac{\partial u_p}{\partial x} \Big|_{x=x_1} dy = 0.
\end{aligned}$$

The integrals along the interface $x = x_0$ cancel because of the interface conditions (2.19); the last integral for $x = x_1$ vanishes as $x_1 \rightarrow +\infty$ because the solution is composed of only exponentially decaying evanescent modes. Therefore, we obtain

$$- \int_{\text{vacuum}} \left[\left| \frac{\partial u_v}{\partial x} \right|^2 + \left| \frac{\partial u_v}{\partial y} \right|^2 - \omega^2 |u_v|^2 \right] dx dy = \int_{\text{PML}} \left[\frac{1}{s_x} \left| \frac{\partial u_p}{\partial x} \right|^2 + s_x \left| \frac{\partial u_p}{\partial y} \right|^2 - s_x \omega^2 |u_p|^2 \right] dx dy.$$

The left-hand side above is real and non-positive since if we represent u_v in the form of the series (2.44a) and take into account that the only terms left are those with $k^2 > \omega^2$, we easily make sure that $\left| \frac{\partial u_v}{\partial y} \right|^2$ dominates over $\omega^2 |u_v|^2$. Dividing both sides by s_x we receive

$$- \frac{\omega \sigma_x}{\sigma_x^2 + \omega^2} \int_{\text{vacuum}} \left[\left| \frac{\partial u_v}{\partial x} \right|^2 + \left| \frac{\partial u_v}{\partial y} \right|^2 - \omega^2 |u_v|^2 \right] dx dy = \frac{2\omega^3 \sigma_x}{(\sigma_x^2 + \omega^2)^2} \int_{\text{PML}} \left| \frac{\partial u_p}{\partial x} \right|^2 = 0.$$

From here we conclude that $\partial u_p / \partial x \equiv 0$ in the infinite PML area and consequently, $u_p \equiv 0$. Therefore, for the vacuum solution u_v we have found that it vanishes along with $\partial u_v / \partial x$ at the interface $x = x_0$. As u_v is analytic, $u_v \equiv 0$, and we have thus shown that the entire homogeneous waveguide solution $u(x, y) \equiv 0$. \square

The next theorem shows uniqueness for the waveguide problem with the PML of finite thickness.

THEOREM 2.11. *Let the PML in the waveguide have finite thickness, $L > x_0$, see Figure 2.3. Let $u = u(x, y)$ satisfy equation (1.5) in the vacuum area of the waveguide, equation (1.4) with $\sigma_x \neq 0$, $\sigma_y = 0$, in the PML area, interface conditions (2.19) at $x_{\text{int}} = x_0$, and be equal to zero, $u = 0$, at $x = 0$, $x = L$, $y = 0$, and $y = \pi$. Then, $u \equiv 0$.*

Proof. We again expand $u(x, y)$ in the sine Fourier series (2.44a) with respect to the transversal coordinate y for each x : $0 \leq x \leq L$. Then, for each $k = 1, 2, \dots$, the k -th Fourier component $\hat{u}(x, k)$ satisfies equation (2.26a) for $0 \leq x \leq x_0$ and equation (2.26b) for $x_0 \leq x \leq L$. As the PML is terminated at $x = L$ with the zero Dirichlet boundary condition, then the analysis similar to the one of Section 2.5 yields the PML solution for every k in the form

$$\hat{u}_p(x, k) = C_1 \hat{u}_p^{(1)}(x, k) + C_2 \hat{u}_p^{(2)}(x, k),$$

where the relations between C_1 and C_2 are given by formulae (2.33). Consequently, the corresponding vacuum solution for the mode k takes the form

$$\hat{u}_v(x, k) = A_1 \hat{u}_v^{(1)}(x, k) + A_2 \hat{u}_v^{(2)}(x, k),$$

where the relations between A_1 , A_2 , and C_1 , C_2 , are given by formulae (2.34) that follow from the interface conditions (2.19) for $x_{\text{int}} = x_0$. For the traveling modes, $k^2 < \omega^2$, we conclude from (2.34b) that

$$\left| \frac{A_1}{A_2} \right| = \exp \left(-2\sqrt{1 - k^2/\omega^2} \sigma_x (L - x_0) \right),$$

which means that the two components, $\hat{u}_v^{(1)}$ of (2.27a) and $\hat{u}_v^{(2)}$ of (2.27b), have different absolute magnitudes as long as $L - x_0 > 0$. On the other hand, the homogeneous Dirichlet boundary condition at $x = 0$ along with the fact that $\sin(ky)$, $k = 1, 2, \dots$, is a full orthogonal system, imply that the sum of these two components $\hat{u}_v(x, k)$ has to be equal to zero at $x = 0$ for each k . Clearly, this requirement cannot be satisfied unless both magnitudes are zero: $A_1 = A_2 = 0$. Thus, we have shown (as previously) that even if the solution $u(x, y)$ is nontrivial, it does not contain traveling modes.

We now apply the same argument as the one used when proving Theorem 2.10. We integrate $\bar{u}\mathbf{L}u$ over the entire area of both vacuum and PML. All boundary integrals drop out because of the zero Dirichlet boundary conditions and we obtain

$$\begin{aligned} \int_{\substack{0 \leq x \leq L \\ 0 \leq y \leq \pi}} (\bar{u}\mathbf{L}u) dx dy = & - \int_{\substack{0 \leq x \leq x_0 \\ 0 \leq y \leq \pi}} \left[\left| \frac{\partial u_v}{\partial x} \right|^2 + \left| \frac{\partial u_v}{\partial y} \right|^2 - \omega^2 |u_v|^2 \right] dx dy + \int_0^\pi \bar{u}_v \frac{\partial u_v}{\partial x} \Big|_{x=x_0} dy - \\ & - \int_{\substack{x_0 \leq x \leq L \\ 0 \leq y \leq \pi}} \left[\frac{1}{s_x} \left| \frac{\partial u_p}{\partial x} \right|^2 + s_x \left| \frac{\partial u_p}{\partial y} \right|^2 - s_x \omega^2 |u_p|^2 \right] dx dy + \int_0^\pi \frac{1}{s_x} \bar{u}_p \left(-\frac{\partial u_p}{\partial x} \right) \Big|_{x=x_0} dy. \end{aligned}$$

As before, the interface integrals cancel because of (2.19). Separating the real and imaginary parts, we again obtain that $\partial u_p / \partial x \equiv 0$ over the PML area, which implies (via the boundary condition at $x = L$) that $u_p \equiv 0$. It then follows that $u_v \equiv 0$ and we have thus proven that $u(x, y) = 0$. \square

3. Numerical Methods. We now describe finite difference approximations to the Helmholtz and PML equations. We then discuss iterative methods to solve the resultant system of equations. We rewrite the Helmholtz equation (1.5) using k for the wavenumber.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + k^2(x, y)u = F \quad (3.1)$$

Let $\phi_{i,j}$ be the numerical approximation to $u(x_i, y_j)$, and $F_{i,j} = F(x_i, y_j)$ be a known function. Define

$$\begin{aligned} \phi_s &= \phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} \\ \phi_c &= \phi_{i+1,j+1} + \phi_{i-1,j+1} + \phi_{i+1,j-1} + \phi_{i-1,j-1} \end{aligned} \quad (3.2)$$

We first consider the Poisson equation, with $k = 0$. An approximation to the Laplacian that uses the nine nearest neighbors is

$$L_h \phi = \frac{A_s \phi_s + A_c \phi_c + A_0 \phi_{i,j}}{h^2} \quad (3.3)$$

In order for the approximation to be second order accurate we require that

$$\begin{aligned} 4A_s + 4A_c + A_0 &= 0 \\ A_s + 2A_c &= 1 \end{aligned}$$

By a straightforward Taylor series expansion and use of the Poisson equation we find that

$$L_h \phi = F + \frac{h^2}{12} (F_{xx} + F_{yy}) + \frac{h^4}{360} (F_{xxxx} + 4F_{xxyy} + F_{yyyy}) + O(h^6) \quad (3.4)$$

For the Helmholtz equation we have that

$$F = -k^2 u + f \quad (3.5)$$

Hence,

$$F_{xx} + F_{yy} = -((k^2u)_{xx} + (k^2u)_{yy}) + f_{xx} + f_{yy}$$

So we can approximate the $O(h^2)$ term in (3.4) on the nine point stencil and get a fourth order accurate approximation to the Helmholtz equation. If we wish a sixth order accurate approximation we need to approximate the $O(h^4)$ term in (3.4). However, this contains fourth derivatives of F and so by (3.5) fourth derivatives of u which requires a larger stencil. If k is constant we can use the equation itself to reduce the order of the derivatives. For simplicity we assume $f = 0$ and so we have the homogenous Helmholtz equation. When k is constant $f = 0$ and then by (3.5)

$$F_{xxxx} + 4F_{xxyy} + F_{yyyy} = -k^2(u_{xxxx} + 4u_{xxyy} + u_{yyyy}) = -k^2\left(\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)(u_{xx} + u_{yy}) + 2u_{xxyy}\right)$$

Using (3.1) and (3.5) this can be reduced to

$$\begin{aligned} F_{xxxx} + 4F_{xxyy} + F_{yyyy} &= -k^2\left(\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)(-k^2u) + 2u_{xxyy}\right) \\ &= k^4(u_{xx} + u_{yy}) - 2k^2u_{xxyy} = -k^6u - 2k^2u_{xxyy} \end{aligned}$$

Now second derivatives and a cross fourth derivative appear which can be approximated on the nine point stencil. We thus have achieved sixth order accuracy on a nine point stencil. This construction is not unique since the $O(h^4)$ term in (3.4) need only be approximated to second order accuracy.

3.1. Finite Difference Approximation. We have shown that for constant coefficients it is possible to construct a sixth order approximation to the Helmholtz equation based on a nine point stencil (see also [6]). However, we are also interested in variable k . Furthermore, it is not clear that one can construct approximations to a Neumann boundary condition that preserves the sixth order accuracy. Hence, we consider fourth order approximations to the Helmholtz equation that use at most nine points.

We wish to have a symmetric stencil. We replace the derivatives by a Padé approximation.

$$\phi_{xx} \sim \frac{D_{xx}}{1 + \frac{h^2}{12}D_{xx}} \quad \text{where} \quad D_{xx}\phi = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2}$$

and similarly for ϕ_{yy} . We then clear fractions and get

$$(D_{xx} + D_{yy} + \frac{h^2}{6}D_{xx}D_{yy})\phi + \left[1 + \frac{h^2}{12}(D_{xx} + D_{yy}) + \frac{h^4}{144}D_{xx}D_{yy}\right]k^2\phi = F. \quad (3.6)$$

The h^4 term can be multiplied by an arbitrary constant γ . Expanding this we get

$$\begin{aligned} & -\frac{10}{3}\phi_{i,j} + h^2\left(\frac{2}{3} + \frac{\gamma}{36}\right)(k^2\phi)_{i,j} + \frac{2}{3}\phi_s + \frac{1}{6}\phi_c \\ & + \frac{h^2}{12}\left(1 - \frac{\gamma}{6}\right)(k_{i+1,j}^2\phi_{i+1,j} + k_{i-1,j}^2\phi_{i-1,j} + k_{i,j+1}^2\phi_{i,j+1} + k_{i,j-1}^2\phi_{i,j-1}) \\ & + \frac{\gamma h^2}{144}(k_{i+1,j+1}^2\phi_{i+1,j+1} + k_{i-1,j+1}^2\phi_{i-1,j+1} + k_{i+1,j-1}^2\phi_{i+1,j-1} + k_{i-1,j-1}^2\phi_{i-1,j-1}) \\ & = B_0F_{i,j} + B_s, s + B_c, c \\ & , s = F_{i+1/2,j} + F_{i,j+1/2} + F_{i-1/2,j} + F_{i,j-1/2} \\ & , c = F_{i+1/2,j+1/2} + F_{i-1/2,j+1/2} + F_{i+1/2,j-1/2} + F_{i-1/2,j-1/2} \\ & B_0 = h^2\left(-\frac{1}{3} + \frac{4\delta}{9}\right) \quad B_s = h^2\left(\frac{1}{3} - \frac{2\delta}{9}\right) \quad B_c = h^2\frac{\delta}{9}. \end{aligned} \quad (3.7)$$

see [8, 16] for further details.

We next generalize this to the case of general variable coefficients

$$\frac{\partial}{\partial x} \left(A \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(B \frac{\partial u}{\partial y} \right) + Cu = F \quad (3.8)$$

where A, B, C are general functions of (x, y) . We have not found a formula that keeps the self-adjoint form and is also fourth order accurate for non-constant A and B . However, in our application A and B are variable only in the PML layer which is artificial and hence the order of accuracy is meaningless. Hence, we construct a formula which conserves the self-adjoint form, is fourth order accurate when A, B are constant but C is variable and is second order accurate for variable A, B, C . This is now a straightforward generalization of our previous formula. Let D^+, D^- be forward and backward difference operators respectively. Then

$$\left[D_x^+ A D_x^- + D_y^+ B D_y^- + \frac{h^2}{12} (D_{yy} D_x^+ A D_x^- + D_{xx} D_y^+ B D_y^-) \right] \phi + \left[1 + \frac{h^2}{12} (D_{xx} + D_{yy}) + \frac{\gamma h^4}{144} D_{xx} D_{yy} \right] C \phi = F$$

Expanding this we get

$$\begin{aligned} & \frac{5}{6} [A_{i+1/2,j}(\phi_{i+1,j} - \phi_{i,j}) - A_{i-1/2,j}(\phi_{i,j} - \phi_{i-1,j})] \\ & + \frac{1}{12} [A_{i+1/2,j+1}(\phi_{i+1,j+1} - \phi_{i,j+1}) - A_{i-1/2,j+1}(\phi_{i,j+1} - \phi_{i-1,j+1})] \\ & + \frac{1}{12} [A_{i+1/2,j-1}(\phi_{i+1,j-1} - \phi_{i,j-1}) - A_{i-1/2,j-1}(\phi_{i,j-1} - \phi_{i-1,j-1})] \\ & + \frac{5}{6} [B_{i,j+1/2}(\phi_{i,j+1} - \phi_{i,j}) - B_{i,j-1/2}(\phi_{i,j} - \phi_{i,j-1})] \\ & + \frac{1}{12} [B_{i+1,j+1/2}(\phi_{i+1,j+1} - \phi_{i+1,j}) - B_{i+1,j-1/2}(\phi_{i+1,j} - \phi_{i+1,j-1})] \\ & + \frac{1}{12} [B_{i-1,j+1/2}(\phi_{i-1,j+1} - \phi_{i-1,j}) - B_{i-1,j-1/2}(\phi_{i-1,j} - \phi_{i-1,j-1})] \\ & + h^2 \left(\frac{2}{3} + \frac{\gamma}{36} \right) C_{i,j} \phi_{i,j} \\ & + \frac{h^2}{12} \left(1 - \frac{\gamma}{6} \right) [C_{i+1,j} \phi_{i+1,j} + C_{i-1,j} \phi_{i-1,j} + C_{i,j+1} \phi_{i,j+1} + C_{i,j-1} \phi_{i,j-1}] \\ & + \frac{\gamma h^2}{144} [C_{i+1,j+1} \phi_{i+1,j+1} + C_{i-1,j+1} \phi_{i-1,j+1} + C_{i+1,j-1} \phi_{i+1,j-1} + C_{i-1,j-1} \phi_{i-1,j-1}] \\ & = B_0 F_{i,j} + B_s, s + B_c, c \end{aligned} \quad (3.9)$$

3.2. Preconditioning. We express the generalized Helmholtz equation in the form where we have divided (1.4) by $-s_x s_y$.

$$-Lu - k^2 u = 0 \quad (3.10)$$

Lu is the finite difference approximation to the generalized Laplacian including the s_x and s_y terms. Hence, in general, L is a complex non-self-adjoint operator. Note: we need not choose $k^2 = \omega^2$. Instead, a portion of ω^2 can be included within the L operator. For simplicity, we shall assume $k^2 = \omega^2$. We shall solve the approximation by a Krylov space iteration with preconditioning. The usual case is that k^2 is larger than the first few eigenvalues and much less than the largest eigenvalue, so $\lambda_1 < k^2 \ll \lambda_N$. In particular we assume that the solution is well resolved so that $kh \ll 1$.

For preconditioning we replace the equation

$$Au = f$$

by

$$PAQv = Pv \quad u = Qv \quad (3.11)$$

We wish to choose P and Q so that the condition number of PAQ is smaller than A while P and Q are relatively easy to invert. Since, it is easier to solve symmetric positive definite (spd) problems by conjugate gradient it would be an additional bonus if PAQ is spd even when A is not.

We assume that the operators L and L^* are easy to invert. Inside the physical domain L is an approximation to the Laplacian and so negative definite. Hence, multigrid can be used to efficiently invert L . Hence, we choose

$$P = (L^*)^{-1} + \frac{1}{k^2} \quad , \quad Q = L^{-1}$$

Note: this requires two inversions of a Laplacian at each stage of the Krylov iteration. Then,

$$PAQ = \left((L^*)^{-1} + \frac{1}{k^2} \right) (L + k^2) \frac{L^{-1}}{k^2} = \left((L^*)^{-1} + \frac{1}{k^2} \right) \left(L^{-1} + \frac{1}{k^2} \right) = \left(L^{-1} + \frac{1}{k^2} \right)^* \left(L^{-1} + \frac{1}{k^2} \right) \quad (3.12)$$

Since PAQ is of the form Z^*Z it is symmetric positive definite. Furthermore, since only L^{-1} and its conjugate appear it is compact.

We thus have converted the complex symmetric and nonpositive equation to a symmetric positive definite matrix that can be solved by conjugate gradient. To see the effect of the preconditioning on the condition number we consider the case $\sigma_x = \sigma_y = 0$ and so $L = L^*$ is an approximation to the Laplacian and $-L$ is positive definite. We denote the eigenvalues of $-L$ by λ_i where λ_i are all positive. They are ordered by $\lambda_1 \leq \lambda_2 \dots$. For finite difference approximations λ_1 is a constant of order 1 while $\lambda_N = O(h^{-2})$. We denote λ_K as the eigenvalue closest to k^2 with $\lambda_K = k^2 + \epsilon$. Since, we assume the problem is non-singular $\epsilon \neq 0$ but it can be positive or negative.

Then the condition number of the canonical Helmholtz equation is

$$\kappa_H = \left| \frac{\lambda_N - k^2}{\lambda_K - k^2} \right| = O\left(\frac{1}{|\epsilon|h^2}\right) \quad (3.13)$$

Denote by μ_i the eigenvalues of $-L^{-1} - \frac{1}{k^2}$. By a power series expansion $|\mu_K| = \frac{1}{\lambda_K} - \frac{1}{k^2} = O\left(\frac{\epsilon}{k^2}\right)$. Similarly, $|\mu_1| = -\frac{1}{\lambda_1} - \frac{1}{k^2} = O(1) + \frac{1}{k^2}$ and $|\mu_N| = -\frac{1}{\lambda_N} - \frac{1}{k^2} = O(h^2) + \frac{1}{k^2}$. Thus, the condition number of $L^{-1} + \frac{1}{k^2}$ is given by $\left| \frac{\mu_1}{\mu_K} \right| = O\left(\frac{k^4}{\epsilon}\right)$ and so is independent of h . Since, the preconditioning PAQ involves the square of this quantity we have

$$\kappa_{PAQ} = O\left(\left(\frac{k^4}{\epsilon}\right)^2\right). \quad (3.14)$$

Thus, this preconditioned matrix has the disadvantage that it depends on ϵ^2 rather than ϵ but has the double advantage of being spd and independent of h .

3.3. Iterative Methods. Based on the previous section we consider multigrid methods for solving the principal part of the PML equations (which can be used as a preconditioner for the full PML) given by

$$\begin{aligned} Au_{xx} + Bu_{yy} &= 0 \\ A &= \frac{s_y}{s_x} \quad B = \frac{s_x}{s_y} \quad s_x = 1 - i\frac{\sigma_x}{k} \quad s_y = 1 - i\frac{\sigma_y}{k} \end{aligned} \quad (3.15)$$

Note that the frequency that appears in A and B is given by k since ω will denote below an iteration parameter. We replace the derivatives by standard second order accurate finite differences. We shall first consider a damped Jacobi iterative method. Then

$$\begin{aligned} \hat{\phi}_{i,j}^{n+1} &= \frac{1}{2} \left[\frac{A}{A+B} (\phi_{i+1,j}^n + \phi_{i-1,j}^n) + \frac{B}{A+B} (\phi_{i,j+1}^n + \phi_{i,j-1}^n) \right] \\ \phi_{i,j}^{n+1} &= \omega \hat{\phi}_{i,j}^{n+1} + (1-\omega)\phi_{i,j} \end{aligned} \quad (3.16)$$

Fourier transforming we get

$$M_{JOR} = 1 - \frac{\omega}{A+B} [A(1 - \cos(\theta)) + B(1 - \cos(\phi))]$$

We shall only consider the case that $\sigma_y = 0$ (i.e. waveguide). Then

$$\begin{aligned} \frac{A}{A+B} &= \frac{s_y^2}{s_x^2 + s_y^2} = \frac{2 - (\frac{\sigma_x}{k})^2 + 2i(\frac{\sigma_x}{k})}{4 + (\frac{\sigma_x}{k})^4} \\ \frac{B}{A+B} &= \frac{s_x^2}{s_x^2 + s_y^2} = \frac{2 + (\frac{\sigma_x}{k})^2 + (\frac{\sigma_x}{k})^4 - 2i(\frac{\sigma_x}{k})}{4 + (\frac{\sigma_x}{k})^4} \end{aligned}$$

For a multigrid smoother we are interested in finding the maximum of $|M_{JOR}|$ for all high frequencies, i.e. when either θ or ϕ is greater than $\frac{\pi}{2}$. Define

$$G = \max_{\frac{\pi}{2} \leq \theta \leq \pi} \max_{\frac{\pi}{2} \leq \phi \leq \pi} |M(\theta, \phi)|$$

Consider

$$M_{JOR}(\theta, 0) = 1 - \frac{\omega A(1 - \cos(\theta))}{A+B} = 1 - \omega(1 - \cos(\theta)) \frac{2 - (\frac{\sigma_x}{k})^2 + 2i(\frac{\sigma_x}{k})}{4 + (\frac{\sigma_x}{k})^4}$$

If $\frac{\sigma_x}{k} = \sqrt{2}$ then $M_{JOR}(\theta, 0) = 1 - \frac{1}{4}\sqrt{2}i\omega(1 - \cos(\theta))$ and so if ω is real then $|M_{JOR}(\theta, 0)| > 1$. Choosing ω complex does not help as can be verified by checking $|M_{JOR}(0, \pi)|$. This is not surprising as it is well known that point methods are not good smoothers when the ratio of the coefficients A and B is too large. Instead we consider a damped implicit Jacobi method. Hence, we replace (3.16) by

$$\begin{aligned} \hat{\phi}_{i,j}^{n+1} &= \frac{1}{2} \left[\frac{A}{A+B} (\hat{\phi}_{i+1,j}^{n+1} + \hat{\phi}_{i-1,j}^{n+1}) + \frac{B}{A+B} (\phi_{i,j+1}^n + \phi_{i,j-1}^n) \right] \\ \phi_{i,j}^{n+1} &= \omega \hat{\phi}_{i,j}^{n+1} + (1 - \omega) \phi_{i,j} \end{aligned} \tag{3.17}$$

Now

$$M_{IJOR}(\theta, \phi) = 1 - \omega \frac{A(1 - \cos(\theta)) + B(1 - \cos(\phi))}{A(1 - \cos(\theta)) + B}$$

However,

$$M_{IJOR}(\frac{\pi}{2}, \phi) = M_{JOR}(\frac{\pi}{2}, \phi)$$

It can again be verified that if $\frac{\sigma_x}{k} > \sqrt{2}$ then $|M_{IJOR}(\theta, \frac{\pi}{2})| > 1$ even with a complex ω . So implicit Jacobi improves the convergence rate for small $\frac{\sigma_x}{k}$ but does not allow larger values of $\frac{\sigma_x}{k}$.

3.4. Hyperbolic Approach. An alternative method to generating multigrid methods is to convert the steady state equation to a hyperbolic equation in (pseudo-time) and then to march this to a steady state using multigrid with the hyperbolic solver as the smoother (see for example [2]). This usually gives a slower convergence rate than converting the steady state to a parabolic equation. However, in many cases it is more robust for a large class of problems. We first consider the first order system for linear acoustics with no mean flow.

$$\begin{aligned} p_t - i\omega p &= c(u_x + v_y) \\ u_t - i\omega u &= cp_x \\ v_t - i\omega v &= cp_y \end{aligned} \tag{3.18}$$

We can convert this to a second order equation for the pressure, p , getting

$$p_{tt} - 2i\omega p_t = c^2 (p_{xx} + p_{yy}) + \omega^2 p \quad (3.19)$$

Assuming $p \sim e^{ikt}$ a straightforward dispersion analysis shows that this equation has plane wave solutions depending on $k + \omega$. We can approximate the first order system using Runge-Kutta in time or the second order equation using central differences in space and time. One usually adds an artificial viscosity or upwinding to remove the high frequency errors.

We next consider a similar procedure for the PML equations. For simplicity we set $c = 1$ and then rewrite (1.2) as

$$\begin{aligned} (i\omega + \sigma_x)(i\omega + \sigma_y)p &= i\omega (u_x + v_y) \\ i\omega(i\omega + \sigma_x)u &= (i\omega + \sigma_y)p_x \\ i\omega(i\omega + \sigma_y)v &= (i\omega + \sigma_x)p_y \end{aligned} \quad (3.20)$$

Beginning with (3.20) we add the time derivative back again to get a smoother in pseudo-time. Thus,

$$\begin{aligned} \left(\frac{\partial}{\partial t} + \sigma_x\right)\left(\frac{\partial}{\partial t} + \sigma_y\right)p + (i\omega + \sigma_x)(i\omega + \sigma_y)p &= \frac{\partial}{\partial t} (u_x + v_y) + i\omega (u_x + v_y) \\ \frac{\partial}{\partial t}\left(\frac{\partial}{\partial t} + \sigma_x\right)u + i\omega(i\omega + \sigma_x)u &= \left(\frac{\partial}{\partial t} + \sigma_y\right)p_x + (i\omega + \sigma_y)p_x \\ \frac{\partial}{\partial t}\left(\frac{\partial}{\partial t} + \sigma_y\right)v + i\omega(i\omega + \sigma_y)v &= \left(\frac{\partial}{\partial t} + \sigma_x\right)p_y + (i\omega + \sigma_x)p_y \end{aligned} \quad (3.21)$$

Assuming σ_x, σ_y are constant we arrive at a sixth order equation for the pressure

$$\begin{aligned} &\left[\frac{\partial}{\partial t}\left(\frac{\partial}{\partial t} + \sigma_x\right) + i\omega(i\omega + \sigma_x)\right] \left[\frac{\partial}{\partial t}\left(\frac{\partial}{\partial t} + \sigma_y\right) + i\omega(i\omega + \sigma_y)\right] \\ &\left[\left(\frac{\partial}{\partial t} + \sigma_x\right)\left(\frac{\partial}{\partial t} + \sigma_x\right) + (i\omega + \sigma_x)(i\omega + \sigma_y)\right] p \\ &= \left(\frac{\partial}{\partial t} + i\omega\right) \left[\frac{\partial}{\partial t}\left(\frac{\partial}{\partial t} + \sigma_y\right) + i\omega(i\omega + \sigma_y)\right] \left[\frac{\partial}{\partial t} + \sigma_y + i\omega + \sigma_y\right] p_{xx} \\ &+ \left(\frac{\partial}{\partial t} + i\omega\right) \left[\frac{\partial}{\partial t}\left(\frac{\partial}{\partial t} + \sigma_x\right) + i\omega(i\omega + \sigma_x)\right] \left[\frac{\partial}{\partial t} + \sigma_x + i\omega + \sigma_x\right] p_{yy} \end{aligned}$$

If we Fourier transform this in time, $p \sim e^{ikt}$, then we recover (1.4) for $k + \omega$.

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