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Perfectly Matched Layers for Second Order Wave Equations

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Abstract

Numerical simulation of propagating waves in unbounded spatial domains is a challenge common to many branches of engineering and applied mathematics. Perfectly matched layers (PML) are a novel technique for simulating the absorption of waves in open domains. The equations modeling the dynamics of phenomena of interest are usually posed as differential equations (or integral equations) which must be solved at every time instant. In many application areas like general relativity, seismology and acoustics, the underlying equations are systems of second order hyperbolic partial differential equations. In numerical treatment of such problems, the equations are often rewritten as first order systems and are solved in this form. For this reason, many existing PML models have been developed for first order systems. In several studies, it has been reported that there are drawbacks with rewriting second order systems into first order systems before numerical solutions are obtained. While the theory and numerical methods for first order systems are well developed, numerical techniques to solve second order hyperbolic systems are less developed.

In the first part of this thesis, we construct PML equations for systems of second order hyperbolic partial differential equations in two space dimensions, focusing on the equations of linear elasto-dynamics. One advantage of this approach is that we can choose auxiliary variables such that the PML is strongly hyperbolic, thus strongly well-posed. The second is that it requires less auxiliary variables as compared to existing first order formulations. However, in continuum the stability of both first order and second order formulations are linearly equivalent. A turning point is in numerical approximations. We have found that if the so-called geometric stability condition is violated, approximating the first order PML with standard central differences leads to a high frequency instability for any given resolution. The second order discretization behaves much more stably. In the second order setting instability occurs only if unstable modes are well resolved.

The second part of this thesis discusses the construction of PML equations for the time-dependent Schrödinger equation. From mathematical perspective, the Schrödinger equation is unique, in the sense that it is only first order in time but second order in space. However, with slight modifications, we carry over our ideas from the hyperbolic systems to the Schrödinger equations and derive a set of asymptotically stable PML equations. The new model can be viewed as a modified complex absorbing potential (CAP). The PML model can easily be adapted to existing codes developed for CAP by accurately discretizing the auxiliary variables and appending them accordingly. Numerical experiments are presented illustrating the accuracy and absorption properties of the new PML model.

We are hopeful that the results obtained in this thesis will find useful applications in time-dependent wave scattering calculations.

List of papers

This thesis is based on the following papers, which are referred in the text by their Roman numerals.

- I K. Duru and G. Kreiss. A well-posed and discretely stable perfectly matched layer for elastic wave equations in second order formulation. Technical report, Division of Scientific Computing, Department of Information Technology, Uppsala University Sweden. ISSN 1404-3203; 2010-004.
- II G. Kreiss and K. Duru. Discrete stability of perfectly matched layers for wave equations in first and second order formulations. To be submitted.
- III K. Duru and G. Kreiss. Stable perfectly matched layers for the Schrödinger equations. Proceedings of ENUMATH 2009, the 8th European Conference on Numerical Mathematics and Advanced Applications. Accepted for publication.

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Chapter 1

Introduction

Many phenomena in biology, engineering and physical sciences can be described by wave motion. Typical examples are aerodynamics, acoustics, electromagnetics, seismology and quantum dynamics. For wave propagating problems, the spatial domain is often very large compared to the characteristic dimension, the wavelength. In numerical simulations, large spatial domains must be truncated to fit into the finite memory of the computer, thereby introducing artificial computational boundaries, as shown in Figure 1.1.

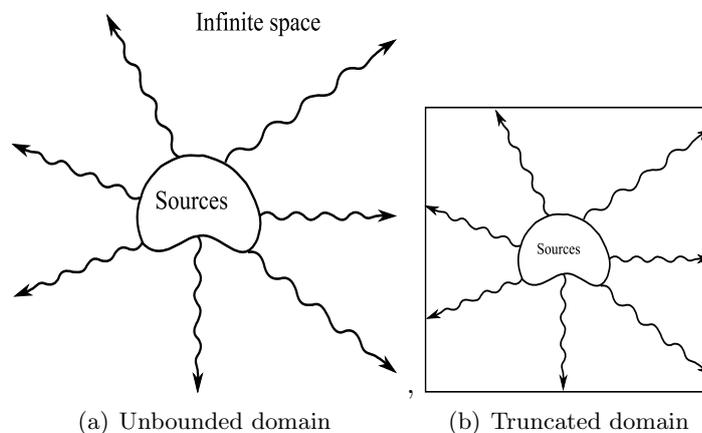


Figure 1.1: A typical set-up: to the left Figure (a), local sources emit waves into the infinite space; to the right Figure (b), the infinite space is truncated to a rectangular computational domain.

One could immediately pose the question:

Which boundary conditions ensure that the numerical solution of the initial-boundary value problem inside the truncated domain converges to the solution of the original problem in the unbounded domain?

Provided the numerical method used in the interior is consistent and stable, the computed solution will converge to the solution of the original problem in the unbounded domain only if artificial boundaries are closed with ‘accurate’ and reliable boundary conditions. Otherwise, waves traveling out of the computational domain generate spurious reflections at the boundaries which will travel back into the computational domain and pollute the solution everywhere. It becomes apparent that the most important feature of artificial boundary conditions is that, all out-going waves should disappear (or are absorbed) without reflections.

In a numerical wave simulator, an efficient artificial boundary condition becomes essential since it enables more accurate simulation of waves in many application areas. One example is in numerical simulation of elastic waves to explore natural minerals in the subsurface, to detect cracks and faults in solid structures or to predict strong ground motions such as earthquakes. Another example is the design for noise reduction in aircrafts¹, and vehicles like cars or trains. The study of dissociative chemical reactions and the design of powerful lasers aided by numerical simulation of the Schrödinger equations are also important application areas.

The effort to design efficient artificial boundary conditions began over thirty years ago and has evolved over time to become an entire area of research. The underlying problem determines the level of difficulty of constructing a particular artificial boundary condition. It is possible to hierarchically classify the underlying problems in increasing order of difficulty as follows: *time-harmonic problems*, *linear time-dependent constant coefficient problems*, *linear time-dependent variable coefficient problems*, *non-linear time-dependent problems*.

Artificial boundary conditions in general can be divided into two main classes: absorbing or non-reflecting boundary conditions (NRBC) and absorbing layers. We also note that for time-harmonic problems there are accurate and efficient artificial boundary procedures, see [72, 36]. Problems of this class are not considered in this thesis.

Most domain truncation schemes for time-dependent wave propagation problems have been developed for constant coefficient wave propagation problems. Many of these methods such as high order local NRBCs and the perfectly matched layer (PML) which we will discuss in Chapter 2 and Chapter 3 respectively, are efficient for certain problems, particularly the scalar wave equation and the Maxwell’s equation in isotropic homogeneous media. For many other problems in this class, such as the linearized magneto-hydrodynamic (MHD) equations and the equations of linear elasticity, there are yet unresolved problems, see for example [15, 9].

Artificial boundary conditions for more difficult problems such as variable coefficient and non-linear wave problems are underdeveloped. In prac-

¹Silent aircraft initiative: www.silentaircraft.org

tice, ad hoc methods are still in use. However, a better understanding of the mathematical properties of the corresponding linear problems will enable the development of efficient boundary conditions for problems of this class.

In this thesis, we consider linear time-dependent constant coefficient wave propagation problems in second order formulation². Our focus is on equations of linear elasticity and the Schrödinger equations. However, with limited modifications the results obtained in this thesis can be applied to other wave equations.

We begin Chapter 2 by illustrating the fundamental ideas underlying the derivation of NRBCs and reviewing some well known results of NRBCs. In Chapter 3, a model problem for second order wave equations is considered, and the PML equations in second order and first order formulations, respectively, are derived. Some of the mathematical properties of the models are also discussed. Chapter 4 is devoted to a short review of absorbing layers for the Schrödinger equations. A summary of the included papers is presented in Chapter 5. In Chapter 6 suggestions for future work are made.

²Note that many linear wave equations that appear as first order systems can be rewritten in second order formulations

Chapter 2

Non-reflecting boundary conditions

The amount of literature on non-reflecting boundary conditions is enormous and constantly increasing. In this section we attempt a brief review of NRBCs for the wave equation. Elaborate discussions can be found in the review papers [72, 30, 35]. A NRBC, as the name implies, is a boundary condition imposed on an artificial boundary to ensure that no (or little) spurious reflections occur from the boundary, see [30]. These boundary conditions can be distinctly classified into: exact (or global) NRBCs, and approximate (or local) NRBCs¹. If a boundary condition is such that the artificial boundary appears perfectly transparent, it is called exact. Otherwise it will correspond to a local (NRBC) approximation and generate some spurious reflections.

2.1 Exact NRBC

To begin, we consider the second order scalar wave equation (2.1) in Cartesian coordinates. The wave equation (2.1) describes pressure waves (or the transverse electric case of the Maxwell's equation) in a homogeneous isotropic media.

$$\begin{aligned} \frac{1}{c^2}u_{tt} &= u_{xx} + u_{yy}, \quad t > 0, \quad (x, y) \in \mathbb{R}^2, \\ u &= u_0, \quad u_t = v_0, \quad t = 0. \end{aligned} \tag{2.1}$$

If we want to compute the solution in the half plane $x < 0$, a NRBC is needed at the artificial boundary $x = 0$, in order to close the statement of the problem and make accurate computations. Exact boundary conditions for (2.1) were first derived in the pioneer work by Engquist and Majda [28] and have recently been reviewed in [30, 35] from a modern perspective. The

¹We note that all exact NRBCs are global, but all global conditions are not exact. Similarly all local NRBCs are approximate but all approximate NRBCs are not local.

construction of the absorbing boundary conditions in [28] uses the fact that any right going solution $u(x, y, t)$ to (2.1) can be represented by a superposition of plane waves traveling to the right. Such solutions are described by

$$u(x, y, t) = e^{-i(\sqrt{(\frac{\omega}{c})^2 - k_y^2}x + \omega t + k_y y)} a_0. \quad (2.2)$$

Here, a_0 is the amplitude of the wave, and (ω, k_y) are the duals of (t, y) , satisfying $\omega^2/c^2 - k_y^2 > 0$ with $\omega > 0$. $\hat{u}(x, k_y, \omega)$ is the wave function in Fourier space. From the argument of Engquist and Majda, the correct boundary condition which annihilates all right going waves at $x = 0$ is

$$\frac{\partial}{\partial x} \hat{u}(x, k_y, \omega) = -i \frac{\omega}{c} \sqrt{1 - (\frac{k_y c}{\omega})^2} \hat{u}(x, k_y, \omega), \quad x = 0. \quad (2.3)$$

Notice that the boundary condition (2.3) is prescribed for $\hat{u}(x, k_y, \omega)$ and not for the time-space dependent wave function $u(x, y, t)$. But $\hat{u}(x, k_y, \omega)$ is related to $u(x, y, t)$ via inverse Fourier transform. Therefore in order to obtain a boundary condition for $u(x, y, t)$ we need to invert the the Fourier transform in (2.3). In theory we can always compute the inverse Fourier transform to determine $\frac{\partial}{\partial x} u(x, y, t)$. Unfortunately, the inverse Fourier transform of (2.3) yields the operator (2.4) which is non-local in both time and space.

$$\frac{\partial}{\partial x} u(x, y, t) = -\mathcal{F}^{-1} \left(i \frac{\omega}{c} \sqrt{1 - (\frac{k_y c}{\omega})^2} \hat{u}(x, k_y, \omega) \right), \quad x = 0, \quad (2.4)$$

$$\text{where } \mathcal{F}^{-1} \hat{u}(x, k_y, \omega) = \int \int e^{i(\omega t + k_y y)} \hat{u}(x, k_y, \omega) dk_y d\omega.$$

This is manifested in the difficulty in inverting the pseudo-differential operator $\sqrt{1 - s^2}$, ($s = k_y c / \omega$) which does not have an explicit local representation. In [28], Engquist and Majda acknowledged this difficulty and instead resorted to some approximations of $\sqrt{1 - s^2}$ which yield a local differential operator upon inversion. The accuracy of the boundary condition then depends on how well $\sqrt{1 - s^2}$ is approximated. As we will see later, this is the basic idea behind local NRBCs.

The contribution [32, 33, 34] by Grote and Keller is another pioneering work in NRBC. Using the Dirichlet to Neumann (DtN) map, Grote-Keller derived the first exact NRBC on a spherical boundary. We note that the Grote-Keller NRBC is inherently three-dimensional, since it is based on special properties of the spherical harmonics. It is believed that no such boundary conditions can be constructed in two space dimensions. This is related to the fact that the Green's function in two-dimensions associated with the wave operator has an infinitely long tail.

Similarly, starting from the Helmholtz equation,

$$\xi^2 \hat{u} = \hat{u}_{xx} + \hat{u}_{yy}, \quad (2.5)$$

Hagstrom [40] used DtN technique to derive the exact boundary condition (2.6) which only involves a Fourier transform in the tangential direction and a convolution in time.

$$K(t) \equiv \frac{J_1(t)}{t} = \frac{1}{\pi} \int_{-1}^1 \sqrt{1-\rho^2} \cos \rho t d\rho,$$

$$\frac{\partial u}{\partial x} + \frac{\partial u}{\partial t} + \mathcal{F}^{-1}(|k_y|^2 K(|k_y|t) * \mathcal{F}u) = 0, \quad x = 0. \quad (2.6)$$

It has been reported that by the use of fast algorithms, together with fast Fourier transform, the boundary condition (2.6) can be directly imposed, see [7].

2.2 Local NRBC

Due to the non-locality of the exact boundary condition (2.3) Engquist and Majda [28] proposed the first hierarchy of local NRBC by replacing $\sqrt{1-s^2}$ with some rational approximation and then inverting the Fourier transform. Approximating $\sqrt{1-s^2}$ by Taylor expansion and including only the first term yields

$$\frac{1}{c} u_t + u_x = 0, \quad x = 0, \quad t > 0. \quad (2.7)$$

This is the so-called first order Engquist-Majda boundary condition. The boundary condition (2.7) remains exact for a two-dimensional wave propagating normal to the boundary. Including the second term of the expansion yields the second order Engquist-Majda boundary condition

$$\frac{1}{c^2} u_{tt} + \frac{1}{c} u_{tx} - \frac{1}{2} u_{yy} = 0, \quad x = 0, \quad t > 0. \quad (2.8)$$

We see that including higher order terms of the Taylor expansion to increase the accuracy of the boundary condition in turn introduces higher order derivatives at the boundary. However, the inclusion of more higher order terms of the the Taylor expansion to improve accuracy of the approximation ceases to yield a well-posed problem. This can be cured by the use of Padé approximations, though. The Padé expansion is not the only possible choice. Other expansions like Chebyshev approximations have been studied. Higdon [45] has a more general representation of these boundary conditions:

$$\left(\frac{\cos \alpha_m}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right) \cdots \left(\frac{\cos \alpha_1}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right) u = 0, \quad x = 0, \quad t > 0, \quad (2.9)$$

where $\alpha_1 \cdots \alpha_m$, are arbitrary parameters. The second order Engquist-Majda boundary condition (2.8) corresponds to $\alpha_1 = 0^\circ, \alpha_2 = 0^\circ$. The higher order derivatives appearing in these boundary conditions greatly complicate

their use in any numerical scheme. As a result, first and second order boundary conditions are most commonly used in practice.

In 1993, Collino [21] introduced a smart idea to remove higher order derivatives while retaining high order accuracy at the boundary. The fundamental idea lies on the approximations of $\sqrt{1-s^2}$, by Padé expansion, and consequently introduce a sequence of auxiliary variables ϕ_j . Collino's idea [21] gave the opportunity to improve the work of Engquist and Majda. Local NRBCs sharing this structure are often referred to as high order local NRBCs, see [30]. Many different high order local NRBCs have been proposed in the past fifteen years, see [30, 41, 37, 72, 30, 35]. The most important property of these high order local NRBCs is that arbitrary order of accuracy can be achieved by introducing more auxiliary variables. In a numerical software the number of auxiliary variables J becomes an input parameter. However, the convergence of the boundary conditions depends on the convergence of the Padé expansion.

Starting from a complete plane wave representation of the time-dependent wave field incorporating both the propagating and evanescent modes, Hagström, et al., derived a new local NRBC [43] that annihilates outgoing waves in both propagative mode and evanescent mode regimes. They also presented strong numerical results indicating the long time efficiency of their model.

The general structure shared by all high order local NRBC is that no high derivatives beyond second order appear, and there are no normal derivatives of any of the auxiliary variables ϕ_j . We point out that on a boundary which has corners, special corner conditions must be used in order for these boundary conditions to yield a well-posed problem.

The major difference between exact NRBCs and approximate NRBCs is that exact NRBCs are non-local in both time and space. Storage requirement remains a drawback for exact NRBCs. Another practical challenge in the implementation of exact NRBCs is the shape of the boundary. The boundary may be very complex such that it becomes extremely difficult to have an explicit representation of the boundary conditions. We also note that while the discussion here is formulated in two space dimensions, the ideas carry over immediately to three space dimensions.

Chapter 3

Absorbing layers for hyperbolic problems

Probably, the most straight forward way to truncate unbounded domains is to surround the computational (truncated) domain with an artificial absorbing layer of finite thickness, see Figure 3.1. All absorbing layers are constructed by modifying the underlying equations such that solutions in the layer decay rapidly. For this method to be effective, it is important that

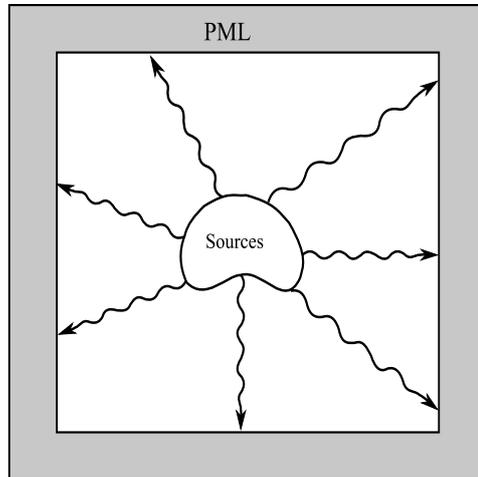


Figure 3.1: A computational domain surrounded by absorbing layers

all waves traveling into the layer, independent of angle of incidence and frequency be absorbed without reflections. This approach is analogous to the physical treatment of the walls of anechoic chambers. Absorbing layers with these desirable features are called perfectly matched layers (PML). By perfect matching we mean that the interface between the computational domain

and the layer exhibits a zero reflection coefficient¹. In practice one takes advantage of this property by reducing the width of the layer dramatically, then choosing the damping coefficient as strongly as possible to minimize the reflections from the edge of the layer. The accuracy of the entire scheme is then determined by the numerical method used in the interior.

The PML was first introduced for the Maxwell's equations by J-P. Bérenger in the seminal paper [14]. Bérenger derived the PML equations by first splitting the wave function into artificial tangential components, then he added a lower order damping term in each normal direction to absorb out-going waves. By rigorously computing the reflecting coefficient of plane waves traveling from the interior into the layer, for arbitrary angles of incidence and frequencies, Bérenger showed that the equations are perfectly matched to the Maxwell's system. Because of the splitting of the Maxwell's equation, Bérenger's PML [14] is called the split-field PML. Independently, Chew and Weedon [18] derived the PML by stretching the spatial coordinates of the Maxwell's equation onto a certain complex contour without introducing the unphysical splitting of the wave function. Another technique to deriving a PML is the use of a modal ansatz introduced by Hagstrom [40]. In general, the PML can be interpreted as a complex change of spatial coordinate of the Fourier (Laplace) transformed wave equation.

Though the main focus of this thesis is on the PML, we also mention that there are other absorbing layers that have been developed, which do not have the perfect matching property. Before the emergence of the PML, Israeli and Orzag [47], Kosloff and Kosloff [50] have began the construction of absorbing layers for wave equations. In a recent work [22, 23], Colonius and Ran proposed an absorbing layer (super-grid scale model) for compressible flow by purely stretching the grid and filtering high frequency components. The paper [10] by Appelö and Colonius extended the work of Colonius and Ran [22, 23] to linear hyperbolic systems. In [27], Efraimsson and Kreiss performed a semi-discrete analysis of a scalar linear model of an absorbing layer (buffer zone). Using their theoretical results Efraimsson and Kreiss suggested how to choose the layer parameters in order to enhance performance, then they applied the result to a full non-linear problem (Euler equations). Unlike the PML, these absorbing layers do not require the use of auxiliary variables. By construction the super-grid scale models [22, 23, 10] are linearly stable. They can be used for non-linear problems where the notion of perfect matching is obscure. However, for linear problems, it is doubtful whether these layers can compete with the PML.

In this chapter, we begin the construction of the PML for a scalar second order model problem. To begin, we introduce a simple model problem for

¹A more general interpretation of perfect matching is that the restriction of the solution to the PML problem in the interior coincides with the solution to the original problem, see [8].

second order strongly hyperbolic systems in two space dimensions. We will then derive a PML model using a plane wave reconstruction that leads to stretching the physical spatial coordinates onto a carefully chosen complex contour, where spatially oscillating solutions are turned into exponentially decaying solutions. The second order model problem will be re-written as a first order system and we will also derive a PML model corresponding to this first order system. Finally, we will comment on perfect matching, well-posedness and stability of the models.

3.1 Model problem

We consider the simple model problem (3.1), the so-called anisotropic scalar wave equation,

$$u_{tt} = u_{xx} + u_{yy} + (\alpha u_y)_x + (\alpha u_x)_y, \quad x, y \in \mathbb{R}, \quad |\alpha| < 1, \quad (3.1)$$

describing electromagnetic waves propagating in an anisotropic dielectric media. If $|\alpha| < 1$, it is easy to show that (3.1) is strongly hyperbolic, see **Paper II**.

3.2 Construction of the PML equations

In this section, we will derive the PML equations. The idea is to introduce new coordinates defined by special complex metrics, see [68, 18]. To begin with, we take Fourier transform in time

$$u(x, y, t) = \int_{-\infty}^{\infty} \hat{u}(x, y, \omega) e^{i\omega t} d\omega,$$

and consider the time-harmonic problem

$$-\omega^2 \hat{u} = \hat{u}_{xx} + \hat{u}_{yy} + (\alpha \hat{u}_y)_x + (\alpha \hat{u}_x)_y. \quad (3.2)$$

The wave equation (3.2) admits plane wave solutions,

$$\hat{u}(x, y, \omega) = u_0 e^{-i\omega(S_x x + S_y y)}.$$

Here S_x and S_y are real, and $(S_x, S_y) = (k_x/\omega, k_y/\omega)$, u_0 is a constant amplitude, (k_x, k_y) is the wave vector.

Let us consider the case where we want to compute the solution in the half plane $x \leq 0$, and the PML is introduced outside that half plane, that is, in $x > 0$. We now look for the modification of the wave equation such that it has exponentially decaying solutions in the PML,

$$\hat{v}(x, y, \omega) = u_0 e^{-S_x \Gamma(x)} e^{-i\omega(S_x x + S_y y)}.$$

Here $\Gamma(x)$ is a real valued non-negative increasing smooth function, which is zero for $x \leq 0$. We can rewrite the decaying solution as

$$\hat{v}(x, y, \omega) = u_0 e^{-i\omega \left(S_x \left(x + \frac{\Gamma(x)}{i\omega} \right) + S_y y \right)}.$$

This can be seen as a plane wave solution to the wave equation in the transformed variables (\tilde{x}, y) , where

$$\tilde{x} = x + \frac{\Gamma(x)}{i\omega}.$$

Since the wave function is analytic, we analytically continue the wave equation (3.2) onto the complex contour \tilde{x} where spatially oscillating solutions are turned into exponentially decaying solutions. We then transform back to real coordinates by applying the following coordinate transformation.

$$\frac{\partial}{\partial \tilde{x}} = \frac{1}{s_1} \frac{\partial}{\partial x}, \quad s_1 := \frac{d\tilde{x}}{dx} = 1 + \frac{\sigma_1}{i\omega}, \quad \text{where} \quad \sigma_1 = \frac{d\Gamma(x)}{dx}. \quad (3.3)$$

The PML is derived by applying this complex change of variables (3.3) in the x -direction, yielding,

$$-\omega^2 \hat{v} = \frac{1}{s_1} \left(\frac{1}{s_1} \hat{v}_x \right)_x + \hat{v}_{yy} + \frac{1}{s_1} (\alpha \hat{v}_y)_x + \left(\alpha \frac{1}{s_1} \hat{v}_x \right)_y. \quad (3.4)$$

$\sigma_1 \geq 0$ is the damping function. We note that in order to enhance the absorption and stability properties of the layer more complicated complex metrics s_1 have been proposed in literature, see [9] and **Paper I**. Notice that the plane wave satisfying (3.4) is

$$\hat{v}(x, y, \omega) = e^{-i\omega(k_1(s_1 x) + k_2 y)} u_0. \quad (3.5)$$

Also note that \hat{u} solves the wave equation (3.2) in the half plane $x < 0$ and \hat{v} is the solution of the PML equation (3.4) in $x > 0$. (3.2) is perfectly coupled to (3.4) with the coupling condition

$$\hat{u}(0, y, s) = \hat{v}(0, y, s), \quad \hat{u}_x(0, y, s) = \hat{v}_x(0, y, s), \quad \sigma_1(0) = 0. \quad (3.6)$$

We localize the PML in time by first introducing the auxiliary variables,

$$\hat{\phi} = \frac{1}{s_1} \frac{\hat{v}_x}{i\omega}, \quad \hat{\psi} = \frac{\hat{v}_y}{i\omega},$$

then inverting the Fourier transforms, yielding

$$\begin{aligned} v_{tt} + \sigma_1 v_t &= v_{xx} + v_{yy} + (\alpha v_y)_x + (\alpha v_x)_y \\ &\quad - (\sigma_1 \phi)_x + (\sigma_1 \psi)_y, \\ \phi_t &= v_x - \sigma_1 \phi, \\ \psi_t &= v_y. \end{aligned} \quad (3.7)$$

3.2.1 First order formulation

In order to demonstrate the construction of the PML for a first order system, we introduce extra variables and rewrite (3.1) as first order system in time and space.

$$\mathbf{u}_t = A\mathbf{u}_x + B\mathbf{u}_y, \quad (3.8)$$

where $A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ \alpha & 0 & 0 \end{pmatrix}$, $B = \begin{pmatrix} 0 & 0 & 1 \\ \alpha & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$.

To derive the corresponding PML model for the first order system (3.8), we apply the complex change of variable (3.3) in the x -direction, then choose the auxiliary variable \mathbf{w} and invert the Fourier transform, we have

$$\begin{aligned} \mathbf{v}_t &= A\mathbf{v}_x + B\mathbf{v}_y - \sigma_1 A\mathbf{w}, \\ \mathbf{w}_t &= \mathbf{v}_x - \sigma_1 \mathbf{w}. \end{aligned} \quad (3.9)$$

Also we comment that the auxiliary variables in (3.7) and (3.9) are zero almost everywhere, except in the layers where $\sigma_1 \neq 0$.

3.2.2 Perfect matching

The most important property of the PMLs (3.7) and (3.9) is that the equations are perfectly matched. This means that the restriction of the solutions to (3.7) and (3.9) in the half plane $x < 0$ coincides with the solutions to (3.1) and (3.8), respectively. There are two standard methods [8, 68] that have been used to study the perfect matching property of the PML. The approach [68] uses plane wave analysis and only accounts for propagating modes. Here, we use the technique [8] which is rooted in the construction of general solution to the wave equation in Laplace-Fourier space. The technique [8] is more general since it includes both the propagating mode regime and the evanescent mode regime. To start with, we take Laplace transform in time $t \rightarrow s$ and Fourier transform in the tangential direction $\partial/\partial y \rightarrow ik_y$. (3.7) and (3.9) are perfectly matched if

$$\begin{aligned} \bar{u}(x, ik_y, s) &= \bar{v}(x, ik_y, s), \quad \text{and} \quad \bar{u}_x(x, ik_y, s) = \bar{v}_x(x, ik_y, s), \quad x \leq 0, \\ \bar{\mathbf{u}}(x, ik_y, s) &= \bar{\mathbf{v}}(x, ik_y, s) \quad x \leq 0. \end{aligned} \quad (3.10)$$

$u, v, \mathbf{u}, \mathbf{v}$ are related to $\bar{u}, \bar{v}, \bar{\mathbf{u}}, \bar{\mathbf{v}}$ via inverse Laplace-Fourier transform. We quickly observe that the perfect matching of the second order PML (3.7) requires the continuity of the solution and its normal derivative across the interface, while the first order PML (3.9) is perfectly matched if only the solutions are continuous across the interface. We can construct modal solutions

$$\bar{u} = e^{\lambda x} \bar{u}_0(s, ik_y), \quad \bar{\mathbf{u}} = e^{\lambda x} \bar{\mathbf{u}}_0(s, ik_y), \quad (3.11)$$

for the problem in the half plane $x \leq 0$, and

$$\bar{v} = e^{\lambda x + \frac{\lambda}{s} \int_0^x \sigma_1(z) dz} \bar{u}_0(s, ik_y), \quad \bar{\mathbf{v}} = e^{\lambda x + \frac{\lambda}{s} \int_0^x \sigma_1(z) dz} \bar{\mathbf{u}}_0(s, ik_y), \quad (3.12)$$

for the PML problem in the half plane $x \geq 0$. Direct calculations show that the first order PML (3.9) is perfectly matched by construction for arbitrary σ_1 , while perfect matching is achieved if $\sigma_1(0) = 0$ in the second order case (3.7). In computations however, additional smoothness at the interface is often beneficial.

Remark 1 *The modal PMLs [40, 9, 8] are derived by first assuming a modal ansatz of the form (3.12). From the modal ansatz the complex metric (3.3) is derived. The PML is then constructed by performing the complex change of variable.*

3.3 Well-posedness

An important mathematical property of a partial differential equation is well-posedness. By a well-posed problem, we mean that there is a unique solution which depends continuously on the data of the problem. To be precise, consider the Cauchy problem

$$\begin{aligned} u_t &= P\left(\frac{\partial}{\partial x}\right)u, \quad x \in \mathbb{R}^n, \quad n \in \mathbb{Z}^+, \quad t \geq 0, \\ u(x, 0) &= u_0(x). \end{aligned} \quad (3.13)$$

Here, the symbol $P\left(\frac{\partial}{\partial x}\right)$ denotes the spatial operator. The Cauchy problem (3.13) is weakly (resp. strongly) well-posed if for every $t_0 \geq 0$,

$$\|u(\cdot, t)\|^2 \leq K e^{\kappa(t-t_0)} \|u_0\|_{H^s}^2,$$

for u_0 giving in the Sobolev space H^s , $s > 0$ (resp. $s = 0$). Here κ and K are independent of u_0 and t_0 .

We demonstrate the well-posedness of the first order and second order PML models (3.9), (3.7). By introducing auxiliary variables we can rewrite (3.7) as a first order system in time and space.

$$U_t = A_1 U_x + A_2 U_y + \sigma_1 A_3 U, \quad (3.14)$$

$$A_1 = \begin{pmatrix} 0 & 1 & 2\alpha & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

It is easy to show that $\forall S = (S_x, S_y) \in \mathbb{R}^2$ normalized to satisfy (3.15)

$$S_x^2 + S_y^2 + 2\alpha S_x S_y = 1, \quad (3.15)$$

the matrix $\hat{A} = S_x A_1 + S_y A_2$ has real eigenvalues and a complete system of eigen-vectors. It follows that the PML model (3.7) is strongly hyperbolic, thus strongly well-posed, see [38]. However, because of the lower order term $\sigma_1 A_3 U$ the system (3.14) may have solutions that grow in time.

Now consider the PML (3.9) for the first order system (3.8). We can rewrite the PML model (3.9) as follows

$$U_t = B_1 U_x + B_2 U_y - \sigma_1 B_3 U, \quad (3.16)$$

$$B_1 = \begin{pmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} \end{pmatrix}, \quad B_2 = \begin{pmatrix} \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad B_3 = \begin{pmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

Since the matrix A in (3.8) has a zero eigenvalue, the matrix $\hat{B} = S_x B_1 + S_y B_2$ is not diagonalizable. Therefore, the PML model (3.9) is weakly (not strongly) hyperbolic, and weakly well-posed. This also is true for the Bérenger's PML.

If we can rewrite (3.1) as a first order system such that the coefficient matrices A and B are invertible it is possible to construct a strongly hyperbolic PML. This is possible for the acoustic (and advective acoustic) wave equations. But for more complex problems such as the elastic wave equations, rewriting the second order system as a first order system will introduce a non propagating mode which will lead to a weakly well-posed PML, see [15, 9].

However, many examples and computations in literature [17, 20, 9, 15] indicate that, for linear constant coefficient problems, loss of strong well-posedness may not be 'disastrous'. We note that if PML models derived for linear constant coefficient problems are to be used for variable coefficient or non-linear problems, it is important that PML equations are strongly well-posed.

3.4 Stability of the PML

For time-dependent problems, it is not sufficient that the PML is well-posed, it must also be stable. By definition well-posed problems support exponentially growing solutions. This is of course undesirable of an absorbing model. The Cauchy problem (3.13) is weakly (resp. strongly) stable if for every $t_0 \geq 0$,

$$\|u(., t)\|^2 \leq K(1 + \gamma t)^s \|u_0\|_{H^s}^2,$$

for u_0 giving in the Sobolev space H^s , with $s > 0$ (resp. $s = 0$). Here K, γ are independent of u_0 and t_0 .

A necessary condition for weak stability is that all eigenvalues λ_j of the symbol $P(i\mathbf{k})$ satisfy

$$\Re \lambda_j(P(i\mathbf{k})) \leq 0.$$

3.4.1 Stability of the continuous PML

In order for the PML to be computationally useful, the PML must be stable. Otherwise any growth in the layer may propagate into the computational domain and pollute the solution everywhere. The question of stability is not trivial, it is therefore a topic of active research.

Perhaps, the earliest reports of (numerical) instabilities in the PML were made in [46, 4]. Applying the split-field PML to the linearized Euler equation, Hu [46] used a filter to ensure that all fields in the layer decay with time. In [4], Abarbanel and Gothlieb performed a mathematical analysis of the Bérenger's PML for Maxwell's equation and found that the PML is only weakly well-posed and under certain perturbations the PML solutions could be inappropriate. Because of the result [4] several unsplit PML were developed [1]. In the paper [3] Abarbanel, et al. studied the longtime stability of these unsplit PML using finite difference methods. The result is that these layers suffer from long time instability due to the Jordan block present in the lower order damping term. Bécache and Joly [17] used standard Fourier techniques and energy methods to establish the well-posedness and stability of the Bérenger's PML for Maxwell's equations. They reported that though Bérenger's PML is weakly well-posed, the damping term appearing in the layer can at the worst lead to a linear growth. In the subsequent paper [16] Bécache, et al. showed that the introduction of the complex frequency shift [54] eliminates the long time instability in the unsplit PML.

While the instability found in [4] is not fatal (since it appear after a very long time), the instability observed in [46] is destructive, and it is inherent in the underlying physical problem. Similar instabilities were also reported for the elastic wave equation in [15]. In the comprehensive stability study [15], Bécache, et. al. established an important but negative stability result. They found that the shape of the slowness curve for an arbitrary first order hyperbolic system determines whether a (continuous) split-field PML can be constructed. It turns out that this is also true for the modal PML, see [9, 8]. In paper **Paper I**, we have also shown that the second order PML for the elastic waves supports growing solutions when this geometric stability condition is violated. However, for some (simple) problems such as (3.1), there are linear transformations which can modify the slowness diagrams such that a stable PML can be constructed, see [12, 24]. For more complex systems like the elastic wave equations such linear transformations may not be possible. We conclude that the stability properties of the continuous first order PML model (3.9) and the second order PML model (3.7) are linearly equivalent. They are in fact unstable if $\alpha \neq 0$. As we commented earlier this problem can be cured by introducing extra terms in the PML which modifies the slowness diagrams, see [12] or introducing such a linear transformation first before the PML is derived [24].

In elastic wave guides, instabilities of the PML have also been reported

when the wave guide is accompanied with free surface or clamped boundary conditions, see [66, 10]. In [66], it was shown that in isotropic elastic wave guides, the PML could be inappropriate when a free surface boundary condition is used along the direction parallel to the wave guide and a PML is used to terminate the wave guide. The explanation is that the free surface boundary conditions support modes with oppositely directed phase and group velocities. In the frequency domain these modes deteriorate the performance of the PML, see [66], while in the corresponding time-domain these modes lead to an exponential growth in the layer, see [10]. In the frequency domain however, Skelton, et al. [66] suggested that the problem could be cured by constructing a frequency-dependent PML with a damping whose sign depends on the frequency. In the time-domain, this problem is yet to be resolved.

3.4.2 Stability of the discrete PML

In literature, very little attention has been paid to the study of stability of discrete PML models. This is in part due to the fact that if a continuous PML model is unstable it may be very difficult to construct accurate and stable discrete approximations. However, in the discrete setting, a finite number of grid points are used and derivatives are also approximated (for example by finite difference). For a given discretization the instability or stability in the continuous model can be strengthened or weakened. A relevant article to this study is the recent work [2]. In this paper [2], Abarbanel, et al. performed a systematic experimental study of the long-time behavior of discrete un-split PML models for the Maxwell's equation. They found that the long-time stability of a given un-split PML also depends on the chosen discrete approximation.

The study of discrete stability of the PML is also a topic of **Paper I, II**.

Chapter 4

Absorbing layers for Schrödinger equation

We consider the appropriately scaled one dimensional linear time-dependent Schrödinger equation,

$$\begin{aligned} iu_t &= Hu, & x \in \mathbb{R}, & \quad t \geq 0, \\ u(x, 0) &= u_0(x), \\ \lim_{|x| \rightarrow \infty} u(x, t) &= 0. \end{aligned} \tag{4.1}$$

The complex valued function $u(x, t)$ is the wave function, $H = -\partial^2/\partial x^2 + V(x, t)$ is the Hamiltonian and $V(x, t)$ is a real potential. The Schrödinger equation (4.1) describes the quantum nature of molecular processes such as chemical reactions. The square modulus of the wave function $|u(x, t)|^2$ called the probability density function gives the likelihood for the system to be in the configuration defined by the spatial variable x at time t .

In order to simulate atoms exposed to intense laser pulse [44] or study chemical dissociation processes [48], one often seeks the numerical solution to the Schrödinger equation (4.1) in a finite computational interval $[-x_0, x_0]$ by introducing artificial computational boundaries $\{\pm x_0\}$. It follows that accurate and reliable boundary conditions are needed at the (artificial) boundaries $\{\pm x_0\}$ in order to close the statement of the problem. The review of such boundary procedures is the focus of this chapter.

In the numerical analysis community, NRBCs for the Schrödinger equations have received a great attention. A recent review of NRBCs for the Schrödinger equations is presented in [13]. The article [13] is quite extensive, highlighting the plethora of work done in this field recently. The use of absorbing layers in open domain simulations of the Schrödinger equation (4.1) has been around in the applied science community. The success of these layers lie in their simplicity. In this chapter, we do not present a detailed survey of this field, rather we aim to point out some of the existing results

our work is based upon. For more elaborate discussions we recommend the articles [59, 62] for a review.

4.1 The complex absorbing potential

The most common approach to constructing absorbing layers for the time-dependent (and time-independent) Schrödinger equation in open domains is the complex absorbing potential (CAP). In order to absorb outgoing waves, see [64, 55, 31, 59], the chemist simply adds a lower order damping term $-i\eta W(x)u(x, t)$ to the right-hand side of the Schrödinger equation (4.1), in a layer of finite width d_0 outside the domain of interest. The initial boundary value problem (4.2) is then solved numerically in a bounded computational domain $[-x_0 - d_0, x_0 + d_0]$. The complex function $-i\eta W(x)$ with strictly negative imaginary part is called CAP. The damping coefficient η is a strictly positive real number. $W(x)$ is a real valued non-negative increasing smooth function, which is zero for $|x| \leq x_0$, ($|W|_\infty = 1$ is in general preferred).

$$\begin{aligned} iu_t &= -u_{xx} + V(x, t)u - i\eta W(x)u, & x \in [-x_0 - d_0, x_0 + d_0], & d_0, t \geq 0, \\ u(x, 0) &= u_0(x), \\ u(-x_0 - d_0, t) &= u(x_0 + d_0, t) = 0. \end{aligned} \tag{4.2}$$

The CAP technique is very popular and has the capability of (partially) damping waves traveling outside the domain of interest if $\eta \gg 1$. This technique is simple, easy to implement in a numerical code and it is compatible with pseudo-spectral methods. However, CAP generates spurious reflections at the interface between the physical domain and the layer which prevents the convergence of the numerical solution for a finite width layer (i.e. not perfectly matched). Because of the simplicity of CAP, efforts have been made to derive optimal CAP parameters, as in the ‘transmission-free’ CAP, see [55]. For a given frequency range $[k_{\min}, k_{\max}]$, the CAP parameters can be tuned to enhance performance. However, for long waves (low frequencies) the performance of CAP depreciates dramatically.

4.2 Smooth exterior scaling and exterior complex scaling

An alternative and a more mathematically rigorous approach to achieving an absorbing boundary for the Schrödinger equation is the smooth exterior scaling (SES) or exterior complex scaling (ECS), see [48, 44, 69, 62]. SES and ECS are very similar in the sense that they depend on the analytic

continuation of the wave function (or scaling the Hamiltonian) on a complex contour,

$$x \rightarrow xe^{i\theta}, \quad (4.3)$$

where $0 < \theta < \pi/2$. Such complex coordinate transformation (4.3) is made outside the domain of interest $[-x_0, x_0]$ such that all out-going waves decay exponentially. This approach is analogous to the PML (which we describe below). The difference between SES and ECS depends on the smoothness of the transition into the complex contour. In the SES technique the real coordinate is smoothly continued into the complex plane, while in the ECS method, the real coordinate is simply rotated into the complex plane. In the continuous setting, because of the smoothness of the transition into the complex contour the interface between the SES and computational domain has zero reflection coefficient. In the ECS case the reflection coefficient is not zero. However, in the discrete setting smoothness of coordinate transformation is necessary in order to minimize numerical reflections.

4.3 Perfectly matched layer for the Schrödinger equation

The PML which also stands on a solid mathematical ground might be a better approach to truncating unbounded domains for the Schrödinger equation. The earliest applications of the PML technology to numerical quantum dynamics can be traced to the papers [19, 6]. However, these PMLs are less analyzed.

A popular approach to deriving PML equations for the Schrödinger equation is the so-called modal ansatz, first introduced by Hagstrom in [40]. The PML model derived with the modal ansatz produces encouraging results for the 1-D linear Schrödinger wave equation with zero or constant potentials. An attempt to extend this model to variable or non-linear potentials in [73] produced unsatisfactory results. This is in part due to the assumptions that there are no variations in the normal direction. Recently, a more thorough study of the convergence properties of the modal ansatz PML has been performed in [61]. One result is that, for a constant potential, the uniform convergence of a numerical method of order p requires a monomial absorbing function of degree $p + 1$. The modal ansatz PML has the advantage of not introducing extra variables in the layer.

In **Paper III**, we studied a new PML which can be viewed as a modified CAP technique. Preliminary calculations show that our layer is not that sensitive to the smoothness of the the absorption function. Unlike the modal PML our PML requires an additional auxiliary variable defined (only) in the layer.

Chapter 5

Summary of papers

This chapter presents the summary of the individual papers included in this thesis. The material contained in this thesis discusses the construction and implementation of the perfectly matched layer for second order wave equations. Our focus is the stability of the perfectly matched layer from the continuous setting to the discrete setting. The sections below briefly describe each paper, also highlight the main results in the papers.

5.1 Paper I

In this paper we derive a PML for the second order formulation of linear, anisotropic elastodynamics in two space dimensions. The layer equations are derived by applying a complex coordinate stretching directly to the second order equations. The resulting system is strongly hyperbolic. By a standard perturbation argument our PML at constant coefficients suffers from the same high frequency instability as the modal PML and the split field PML if the geometric stability condition is violated, while the complex frequency shift has a stabilization effect. However, in computations using standard second order finite differences our PML behaves much better than a standard first order PML. We have found several reasons for this.

In a discrete setting the unstable modes may be of higher frequency than can be represented, or well represented, on the grid. The temporal behaviour of such modes cannot be expected to be predicted by continuous analysis. We also show that this effect can be enhanced by coordinate compression in the layer. However, coordinate compression increases the stiffness of the problem.

Secondly, we observe that the geometric instability gives rise to growing modes, with bulk localized to part of the layer, and propagating tangentially. If a Cartesian domain is surrounded by layers, the bulk of the unstable mode eventually moves into a corner region, and decays. We analyze the stability properties of the corner region as before, finding that there is no

high frequency instability. We have also observed that even if the geometric stability condition is severely violated, on a reasonably fine mesh the discrete PML is stable.

5.2 Paper II

In **Paper I**, numerical experiments using standard second order central finite differences for anisotropic elastodynamics demonstrate that the PML in first order formulation is very sensitive to high frequency instability. The corresponding second order formulation behaves dramatically better. In this paper we investigate this observation from a theoretical point of view. The result is that, if the so-called geometric stability condition is violated, the spurious modes introduced by a straight-forward discretization of the first order formulation lead to high frequency instability for any given resolution. In the corresponding second order discretization the PML is unstable only if unstable modes are not well resolved. Several numerical experiments are presented which confirm the theoretical results.

5.3 Paper III

Perfectly matched layers for the time-dependent Schrödinger wave equations are derived and analyzed. Using plane waves and standard perturbation techniques we show that the solutions in the PML decay exponentially in time and the direction of increasing damping. Numerical experiments are presented, illustrating the perfect matching and absorption properties of the new model. The new model can be viewed as a modified CAP technique, where the Hamiltonian is perturbed by a CAP and the equations are corrected by carefully chosen auxiliary functions to ensure that the interface between the PML and the physical domain has a zero reflection coefficient. Since CAP reflects out-going waves, a lot of effort has been made to derive optimal CAP parameters. These derived optimal parameters can be used in the new PML model to improve results of numerical simulations.

Chapter 6

Future work

In this thesis, the study of continuous and discrete stability of the PML for hyperbolic problems has been of particular interest. In the continuous setting the stability of the PML can be predicted by the geometric stability condition [15], while in the discrete setting, the second order PML is unstable only if unstable modes are well resolved **Paper I, II**. We must note that the analysis yielding the geometric stability condition assumes periodicity of the solution in all directions. If the problem is not periodic in one or more directions other techniques are needed. This is typical of waveguides. For example the instability reported in [66, 10] can not be directly explained by the geometric stability condition. Since the instability [66, 10] appear only when certain boundary conditions accompany the waveguide, it will also be of interest to analyze the PML in a waveguide as an initial boundary-value problem (including the physical boundary conditions) and hopefully propose a cure for this problem.

In practice we often encounter discontinuous interfaces arising either from variations of numerical grid density or from the variations of the underlying media such as a layered elastic media. For the PML to be applied to these problems it will be useful to understand the behavior of the PML in the vicinity of such interfaces. We hope to begin this investigation in the near future.

The PML for the Schrödinger equation presented in **Paper III** is still under development. We hope to further study the properties such as modeling error, discrete reflection coefficient and try to optimize the layer parameters in order to enhance performance.

Finally, the PML which is of course a numerical tool must be included in a powerful numerical software to simulate realistic physical problems. Such softwares make use of massive parallel computers and take advantage of modern computer architecture. We hope to develop a recipe in the finite difference setting to make the coupling of the PML to numerical softwares efficient. The procedure must be numerically stable and must ensure that

all variables in the PML are local such that the interior scheme can be developed in the absence of the PML.

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