Applications of the perfectly matched layers in a discontinuous fluid media

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Abstract

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In this thesis we study the applications of the PML in a multi-layered media. The PML is constructed for the scalar wave equation and the convergence and stability of the continuous problem is studied using the normal mode analysis. A high order accurate semi-discrete problem is constructed by approximating the spatial derivatives with high order finite difference operators satisfying the summation-by-parts properties. To have a stable semi-discrete approximation of the problem, we impose boundary conditions as well as interface conditions using the simultaneous approximation term technique. In order to gain accuracy, a transformed interface condition is constructed for the PML. The semi-discrete problem is approximated using second order accurate central difference scheme. To achieve higher order accuracy we modify the time marching scheme to eliminate truncation errors. Numerical experiments are presented showing that using the proposed transformed interface conditions, higher order of accuracy and convergence are achieved.
1 Introduction

In this thesis, we consider the perfectly matched layers (PML) for wave equations in a discontinuous media. Wave propagation problems are mostly formulated in an unbounded media. When numerical methods such as finite difference methods are used to solve these problems, the domain must be truncated to a bounded domain with artificial boundary conditions. One major problem to this approach is that numerical reflections can be introduced into the solution. A suitable approach for domain truncation is the perfectly matched layer (PML) [1, 2, 6, 12]. The PML is an absorbing layer placed around the computational domain which absorbs outgoing waves. The perfect matching property implies that no reflection is introduced into the computational domain as the waves penetrate the PML.

An efficient way to numerically solve wave propagation problems is to use a high-order accurate spatial scheme with a high-order accurate time marching method [7, 10]. Also to have an accurate numerical method for initial boundary value problems (IBVP), the boundary conditions must be accurately imposed. The SBP-SAT scheme is a stable technique to couple boundary conditions when using finite difference methods [3, 7, 9, 10, 11]. The SBP operators are finite difference operators that satisfy the summation-by-parts (SBP) properties. The simultaneous approximation term (SAT) is a method to impose boundary conditions weakly using penalty terms [3, 11]. The SAT method is also used for numerical interface treatment for wave propagation in discontinuous medias [11].

In theory the PML is a continuous unbounded layer surrounding the computational domain. However, when numerical methods are used, the PML changes to a discrete, finite width layer. In the discrete setting, in order to ensure accuracy and discrete stability, extra care should be taken when using the PML. For instance, if there are physical boundaries extending into the PML, the underlying boundary conditions must also be extended from the physical domain into the PML [4].

The PML and other artificial boundary conditions are often constructed by assuming a homogeneous and infinite media. However, real media are heterogeneous or discontinuous. For example in underwater acoustics it is relevant to consider waveguides consisting of several layers such as air, water, soft and hard sediment and bedrock layers. Applications arising in geophysics and electromagnetic problems can be composed of layers of rock, water and possibly oil.
The ultimate goal of the project is to investigate the efficiency of the PML in a layered fluid media. We are particularly interested in computational set-ups comprising of multi-block domains. The set-up consists of smaller structured domains that are patched together to a global domain using the SBP-SAT technology.

Here, we consider the scalar wave equation in a discontinuous media. We derive interface conditions and formulate a SBP-SAT approximation. Using the energy method, we derive sharp estimates of the penalty parameters, thus proving strict stability. We derive the PML and the corresponding modified interface conditions. Stability of the continuous PML is proven by a modal ansatz. In the discrete setting our modified interface conditions are crucial in order to ensure accuracy.

The outline of the paper is as follows. In section two, we introduce a 1D model problem and the needed background. In section three, we consider a wave propagation problem in a discontinuous media. We derive the interface conditions such that the continuous problem is stable. We construct the semi-discrete approximation of the problem using the SBP-SAT scheme. We prove the discrete stability of the method by deriving sharp estimates for the penalty parameters. In section four, the PML is constructed for 2D wave equation in a discontinuous media. In the continuous setting, the stability of the PML is proven for both homogeneous and discontinuous media. We also modify the interface conditions and extend them to the auxiliary variables. In section five, we construct stable semi-discrete approximation of the PML. We also construct the fully discrete problem for the PML. The numerical experiments are presented in section six. We use the SBP operators used in [4] for our experiments. We start by verifying the accuracy of the interface treatment. We continue to study the accuracy of the PML. We summarize the thesis in the last section.

2 Background

In this section we consider the scalar wave equation in a homogenous fluid media with homogeneous Neumann boundary conditions. We will show well-posedness and stability using the energy method. We will introduce SBP operators and derive strictly stable numerical boundary treatments using the simultaneous approximation term (SAT) method.

The scalar wave equation in a homogenous fluid media is

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} u(x, t) = \frac{\partial^2}{\partial x^2} u(x, t), \quad x \in (0, 1),$$

(2.1)
subject to initial conditions

\[ u(x,0) = f_1(x), \quad \frac{\partial}{\partial t} u(x,0) = f_2(x). \]  

(2.2)

The boundary conditions are

\[ \frac{\partial}{\partial x} u(0,t) = 0, \quad \frac{\partial}{\partial x} u(1,t) = 0. \]  

(2.3)

Note that \( f_1(x) \) and \( f_2(x) \) are smooth functions compactly supported in \((0,1)\). The wave equation (2.1) can describe acoustic wave propagation in fluids. Here \( u \) is the acoustic pressure and \( c \) is the speed of sound.

### 2.1 Well-posedness and stability

To begin, we define the energy

\[ E(t) = \left\| \frac{1}{c} \frac{\partial u}{\partial t} \right\|^2 + \left\| \frac{\partial u}{\partial x} \right\|^2. \]  

(2.4)

In RHS of (2.4), the first term is the kinetic energy and the second term is the potential energy. We multiply (2.1) by \( \frac{\partial u}{\partial t} \) and integrate over \((0,1)\), we have

\[ \frac{\partial}{\partial t} \int_0^1 \left( \frac{1}{c} \frac{\partial u}{\partial t} \right)^2 \, dx = \int_0^1 \frac{\partial u}{\partial t} \frac{\partial^2 u}{\partial x^2} \, dx. \]  

(2.5)

Using integration by parts on the RHS of (2.5), we have

\[ \frac{\partial}{\partial t} \int_0^1 \left( \frac{1}{c} \frac{\partial u}{\partial t} \right)^2 \, dx = - \frac{\partial}{\partial t} \int_0^1 \left( \frac{\partial u}{\partial x} \right)^2 \, dx + \frac{\partial u}{\partial t} \frac{\partial^2 u}{\partial x^2} \bigg|_0 \]  

\[ \Leftrightarrow \frac{\partial}{\partial t} \left( \left\| \frac{1}{c} \frac{\partial u}{\partial t} \right\|^2 + \left\| \frac{\partial u}{\partial x} \right\|^2 \right) = \frac{\partial u}{\partial t} \frac{\partial^2 u}{\partial x^2} \bigg|_0 = 0, \]  

(2.6)

\[ \Leftrightarrow E(t) = E(0). \]  

(2.7)

The energy is conserved. That is the solution \( u \) is uniformly bounded by the initial data for all \( t > 0 \). Thus the problem (2.1) is well-posed and stable.

### 2.2 Summation By Parts operators

Consider the computational domain \( x \in [0,1] \). Let the grid in the x coordinate be defined by

\[ x_j = jh, \quad j = 0, 1, \cdots N - 1, N, \quad h = \frac{1}{N-1}, \]  

(2.9)

where \( N \in \mathbb{N} \) and the grid function is a vector \( v \) of length \( N \).
Let $D_1, D_2$ be discrete operators approximating the first and the second derivatives respectively, that is

$$D_1 \approx \frac{\partial}{\partial x}, \quad D_2 \approx \frac{\partial^2}{\partial x^2}.$$  \hfill (2.10)

The discrete operators $D_1, D_2$ are summation-by-parts (SBP) operators if they satisfy the following properties

$$D_1 = H^{-1}Q, \quad Q^T + Q = B, \quad B = \text{diag}(-1, 0, 0, \ldots, 1), \quad (2.11)$$

$$D_2 = H^{-1}(-M + BS), \quad M = M^T, \quad v^T M v \geq 0, \quad (2.12)$$

$$H = H^T, \quad v^T H v > 0. \quad (2.13)$$

Here $v$ is a vector of length $N$, $Q$ is almost a skew-symmetric operator, $M$ is called the symmetric part of the operator $D_2$ and the operator $S$ is a one sided approximation of the first derivative $\partial/\partial x$ on the boundaries. $H$ defines a discrete norm, $\|v\|_H = v^T H v$. Note that if $H = h I$ (where $I$ is the identity matrix) we get the standard discrete norm. Also note that there exists SBP operators if the computational domain is unbounded but the structure of these operators defer from the description above.

Discrete operators satisfying the summation-by-parts properties (2.11), (2.12), (2.13) are usually derived using $2r$-order ($r = 1, 2, \ldots$) centered difference schemes away from the boundaries and lower order schemes (usually of order $r$) close to the boundaries. The operator $H$ can be a diagonal norm or a block norm. In our experiments we will use the diagonal norm SBP operators.

2.2.1 Semi-discrete approximation (SBP+SAT)

Here we will discretize the wave equation (2.1) using SBP operators and numerically impose the boundary condition (2.3) using the SAT method. The semi-discrete approximation is strictly stable if the discrete equations satisfy discrete energy estimates similar to energy estimate (2.8) of the continuous problem. Strict stability is very important if longtime calculations are required.

Consider the IBVP problem (2.1) subject to the initial condition (2.2) and boundary conditions (2.3). The semi-discrete approximation using the SBP-SAT scheme is

$$\frac{1}{c^2} \frac{d^2 v}{dt^2} = D_2 v - \tau H^{-1} BS v, \quad (2.14)$$

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where $D_2$ is the SBP operator (2.12), (2.13) and $\tau$ is the penalty term. We define discrete energy

$$E(t) = \left\| \frac{1}{c} \frac{\partial \mathbf{v}}{\partial t} \right\|_H^2 + \mathbf{v}^T M \mathbf{v}. \quad (2.15)$$

Substituting the SBP operator $D_2$ in (2.14) and setting $\tau = 1$ we have

$$\frac{1}{c^2} \frac{d^2 \mathbf{v}}{dt^2} = -H^{-1} M \mathbf{v}. \quad (2.16)$$

Multiplying (2.16) by $(d\mathbf{v}/dt)^T H$ and adding the transpose of the products we have

$$\frac{d}{dt} E = 0, \quad (2.17)$$

$$\iff E(t) = E(0). \quad (2.18)$$

The discrete approximation (2.14) is strictly stable.

### 3 Discontinuous media

In this section we will consider the wave equation in a discontinuous media. We will derive interface conditions. We will derive a SBP-SAT semi-discrete approximation and prove stability by deriving sharp estimates of the penalty terms for SBP operators with different order of accuracy.

The discontinuity in the media is reflected on the underlying system of equations by changes (jumps) in the velocity coefficient. We consider 1D scalar wave equation in a domain consisting of two materials coupled at $x = 0$, the system of equations is

$$\frac{1}{c_1^2} \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \quad x \in \Omega_1 = (-\infty, 0) \quad (3.1)$$

$$\frac{1}{c_2^2} \frac{\partial^2 v}{\partial t^2} = \frac{\partial^2 v}{\partial x^2} \quad x \in \Omega_2 = (0, \infty) \quad (3.2)$$

$$u(0, x) = f_1(x), \frac{\partial}{\partial t} u(0, x) = g_1(x) \quad (3.3)$$

$$v(0, x) = f_2(x), \frac{\partial}{\partial t} v(0, x) = g_2(x), \quad (3.4)$$

subject to the initial conditions (3.3) and (3.4). Here $c_1$ and $c_2$ are the wave speeds and $f_1(x), f_2(x), g_1(x)$ and $g_2(x)$ are smooth functions.

At $x = 0$ we need a relation between $u$ and $v$ in order to compute the
solution. This conditions are called physical interface conditions. We will use
\[
\begin{aligned}
    u = v, \\
    c_1^2 \frac{\partial u}{\partial x} = \frac{c_2}{2} \frac{\partial v}{\partial x},
\end{aligned}
\] (3.5)
as our interface conditions. Physically, the first condition corresponds to the equality of the acoustic pressures while the second condition express that the flux of the waves should be the same on the interface.

We show that using the proposed interface conditions (3.5), the energy estimate can be derived thus proving that the problem is well-posed.

To begin, We define the energy as
\[
E = \left\| \frac{\partial u}{\partial t} \right\|_{\Omega_1}^2 + \left\| c_1 \frac{\partial u}{\partial t} \right\|_{\Omega_1}^2 + \left\| \frac{\partial v}{\partial t} \right\|_{\Omega_2}^2 + \left\| \frac{c_2}{2} \frac{\partial v}{\partial x} \right\|_{\Omega_2}^2.
\]

Multiplying (3.1) by \(u_t\) and (3.2) by \(v_t\) and integrating over the domain we have
\[
\frac{d}{dt} \left( \left\| \frac{\partial u}{\partial t} \right\|_{\Omega_1}^2 + \left\| c_1 \frac{\partial u}{\partial t} \right\|_{\Omega_1}^2 \right) = 2c_1 \left( \frac{\partial u}{\partial t} \right) |_{\Omega_1}^0 - \int_{\Omega_1} c_1 \frac{\partial^2 u}{\partial t \partial x} \frac{\partial u}{\partial x} dx \quad \text{(integration by parts)}
\]

\[\Rightarrow \frac{d}{dt} \left( \left\| \frac{\partial u}{\partial t} \right\|_{\Omega_1}^2 + \left\| c_1 \frac{\partial u}{\partial t} \right\|_{\Omega_1}^2 \right) = 2c_1 \left( \frac{\partial u}{\partial t} \right) |_{\Omega_1}^0. \quad (3.6)\]

In the same manner for \(v\) we have
\[
\Rightarrow \frac{d}{dt} \left( \left\| \frac{\partial v}{\partial t} \right\|_{\Omega_2}^2 + \left\| \frac{\partial v}{\partial t} \right\|_{\Omega_2}^2 \right) = -2c_2 \left( \frac{\partial v}{\partial t} \right) |_{\Omega_2}^0. \quad (3.7)
\]

Adding (3.6) and (3.7) together we have
\[
\frac{d}{dt} E = 2c_1 \left( \frac{\partial u}{\partial t} \right) |_{\Omega_1}^0 - 2c_2 \left( \frac{\partial v}{\partial t} \right) |_{\Omega_2}^0.
\]

Using the interface conditions (3.5) we have
\[
\frac{d}{dt} E = 0 \iff E(t) = E(0).
\]

The energy is conserved and the problem is well-posed.
3.1 Semi-discrete approximation

We use the SBP-SAT scheme introduced in section 2.2 and impose interface conditions weakly. To simplify, we consider a homogeneous medium with, \( c_1 = c_2 \) and an artificial interface at \( x = 0 \). The semi-discrete approximation using the SBP-SAT scheme is

\[
\begin{align*}
\mathbf{w}_{tt} &= D_{xx} \mathbf{w} - \tau_N \mathbf{H}^{-1} \mathbf{B} D_x \mathbf{w} - \gamma_N \mathbf{H}^{-1} D_x^T \mathbf{B}^T \mathbf{w} + \\
&\quad - \tau_0 \mathbf{H}^{-1} \mathbf{B} \mathbf{w} - \tau_1 \mathbf{H}^{-1} \mathbf{B} \mathbf{w}_t,
\end{align*}
\]

(3.8)

where \( \mathbf{w}, D_{xx}, \mathbf{B}, \mathbf{H} \) and \( D_x \) are defined as

\[
\begin{align*}
\mathbf{w} &= \begin{pmatrix} u \\ v \end{pmatrix}, & \tilde{\mathbf{B}} &= \begin{pmatrix} 0 & 0 \\ 0 & \hat{\mathbf{P}} \end{pmatrix}, & \hat{\mathbf{P}} &= \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \\
D_{xx} &= \begin{pmatrix} D_2 & 0 \\ 0 & D_2 \end{pmatrix}, & \hat{\mathbf{B}} &= \begin{pmatrix} 0 & 0 \\ 0 & \hat{\mathbf{P}} \end{pmatrix}, & \hat{\mathbf{P}} &= \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, \\
D_x &= \begin{pmatrix} D_1 & 0 \\ 0 & D_1 \end{pmatrix}, & \mathbf{H} &= \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix}.
\end{align*}
\]

(3.9), (3.10), (3.11)

In (3.8) the first term in the right hand side is the discrete approximation of \( \partial^2 \mathbf{w} / \partial x^2 \), the second term is discrete imposition of the interface condition \( c_2^2 (\partial u / \partial x) = c_2^2 (\partial v / \partial x) \), the third and fourth term impose \( u = v \) and the last term imposes \( \partial u / \partial t = \partial v / \partial t \).

Note that \( \tilde{\mathbf{B}} \) is zero everywhere except on the interface, that is \( (\tilde{\mathbf{B}} \mathbf{w})_i = 0, i \notin \{N, N+1\} \), \( (\tilde{\mathbf{B}} \mathbf{w})_N = \mathbf{u}_N - \mathbf{v}_0 \) and \( (\tilde{\mathbf{B}} \mathbf{w})_{N+1} = \mathbf{v}_0 - \mathbf{u}_N \). Also note that \( \mathbf{0} \) is a zero matrix.

3.2 Stability

We analyze the stability of the numerical interface treatment (3.8) for 2nd, 4th and 6th order accurate SBP operators. The aim is to derive sharp estimates of the penalty terms \( \tau_0, \tau_N, \tau_1, \gamma_N \) such that we have an energy estimate. Note that these estimates are sharp, meaning that if values smaller than these estimates are used our semi-discrete approximation becomes unstable. To begin with, we need some definitions and theorems.

**Definition 1** (Gershgorin disc). Let \( A \) be a complex \( n \times n \) matrix, with entries \( a_{ij} \). For \( 1 \leq i \leq n \) let \( R_i = \sum_{j=1, j \neq i}^{n} |a_{ij}| \) be the sum of the absolute values of the non-diagonal entries in the \( i \)th row. Let \( D(a_{ii}, R_i) \) be the closed disc centered at \( a_{ii} \) with radius \( R_i \). Such a disc is called a Gershgorin disc.

**Theorem 1** (Gershgorin theorem). Every eigenvalue of \( A \) lies within at least one of the Gershgorin discs \( D(a_{ii}, R_i) \).
Proof. See [8]

**Theorem 2.** Let $A$ and $B$ be symmetric matrices, let $\lambda_i(A)$ denote the $i_{th}$ eigenvalue, where we order the eigenvalues in increasing order. If $\lambda_i(B)$ is nonnegative and $A$ is positive definite, then

$$\lambda_i(BA) \geq \lambda_{\min}(B)\lambda_i(A)$$

Proof. See [5].

We start by replacing $D_{xx}$ with the definition of the SBP operator for second derivative. We also put $\tau_N = \frac{1}{2}$ and $\gamma_N = -\frac{1}{2}$ and simplify, then (3.8) can be rewritten as

$$w_{tt} = H^{-1} \begin{pmatrix} -M & 0 \\ 0 & -M \end{pmatrix} w + \frac{1}{2} H^{-1} \tilde{B} D_x w + \frac{1}{2} H^{-1} D_x^T \tilde{B}^T w$$

$$- \tau_0 H^{-1} \tilde{B} w - \tau_1 H^{-1} \tilde{B} w_t,$$

Here $w$ and $D_x$ are the same as in (3.9) and (3.11). We introduce two matrices

$$Q = \tilde{B} D_x - \tau_0 \tilde{B}$$

$$\tilde{M} = \begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix} - \frac{1}{2} (Q + Q^T).$$

The semi-discrete problem becomes

$$w_{tt} = -H^{-1} \tilde{M} w - \tau_1 H^{-1} \tilde{B} w_t.$$  (3.14)

**Lemma 1.** Consider the matrix $\tilde{M}$ and $Q$ defined in (3.13) and (3.12). If $Q$ can be written as $Q = -BA$ where the matrix $\tilde{B}$ is defined in (3.9) and the matrix $A$ is symmetric positive definite then $\tilde{M}$ is symmetric positive semi-definite.

Proof. We know that $\tilde{B}$ is symmetric positive semi-definite and $A$ is symmetric positive definite, hence by Theorem 2 we have $\lambda_i(BA) \geq 0$.

We know that $\tilde{B} A + (\tilde{B} A)^T$ is symmetric and since it has positive eigenvalues, it is positive semi-definite. We conclude that $Q + Q^T$ is negative semi-definite. From the definition of SBP operators we know that

$$\begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix}$$

is symmetric positive semi-definite, therefore $\tilde{M}$ is symmetric positive semi-definite.
Lemma 2. Consider the system of ODEs (3.14). If $\widetilde{M}$ is symmetric positive semi-definite and $\tau_1 \geq 0$ then

$$E_w(t) = \|w_t\|_H^2 + w^T \widetilde{M} w$$

is a semi-discrete energy and

$$E_w(t) = E_w(0) - \int 2\tau_1 w_t^T \widetilde{B} w_t \, dt.$$  

(3.16)

Therefore the semi-discrete approximation (3.14) is stable.

Proof. We start by multiplying (3.14) by $w^T \widetilde{H}$ from left. We have

$$w_t^T \widetilde{H} w_{tt} = -w_t^T \widetilde{M} w - \tau_1 w_t^T \widetilde{B} w_t.$$  

(3.17)

Taking the transpose of (3.17) we have

$$w_{tt}^T \widetilde{H} w_t = -w_t^T \widetilde{M} w_t - \tau_1 w_t^T \widetilde{B} w_t.$$  

(3.18)

Adding (3.17) and (3.18) we get

$$\frac{dE}{dt} = -2\tau_1 w_t^T \widetilde{B} w_t.$$  

(3.19)

choosing $\tau_1 \geq 0$ we see that the energy is bounded. Note that if $\tau_1 = 0$ we have the equality $E_w(t) = E_w(0)$ and the energy is conserved and when $\tau_0 > 0$, the energy decays. \hfill \square

Next we will show that $Q = -\tilde{B}A$ for 2nd, 4th and 6th order accurate SBP operators. We will also determine sharp estimates of $\tau_0$ such that $A$ is symmetric positive definite. This immediately leads to stability of (3.14) by Lemma 2.

Second order accurate SBP operator We consider the second order SBP operator. Note that for this we define $D_x$ as

$$S = \frac{1}{h} \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}, \quad D_x = \begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}.$$  

(3.20)

We replace $D_x$ in (3.12). We have

$$Q = \tilde{B} D_x - \tau_0 \tilde{B} = \frac{1}{h} \begin{pmatrix} 0 & -1 & 1 & -1 & 1 & 0 \\ -1 & 1 & -1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} - \tau_0 \begin{pmatrix} 0 & 1 & -1 & 0 \\ 1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$  

(3.21)
where $0$ is a zero matrix. We have

$$
(Qw)_N = \frac{1}{h} (u_{N-1} + u_N - v_0 + v_1) - \tau_0 (u_N - v_0)
$$

$$
(Qw)_{N+1} = -(Qw)_N
$$

Setting $\tau_0 = \frac{\tau_0'}{h}$, we have

$$
(Qw)_N = \frac{1}{h} \left( u_{N-1} + u_N - v_0 + v_1 - \tau_0' u_N + \tau_0' v_0 \right) = - \frac{1}{h} \left( u_{N-1} + \tau_0' u_N + v_0 \right) + \frac{1}{h} \left( u_N + \tau_0' v_0 + v_1 \right) .
$$

and

$$
(Qw)_{N+1} = \frac{1}{h} \left( u_{N-1} + \tau_0' u_N + v_0 \right) - \frac{1}{h} \left( u_N + \tau_0' v_0 + v_1 \right) .
$$

We can write $Q$ as

$$
Q = -BA, \quad A = \begin{pmatrix}
\tau_0' & 1 & & \\
1 & \tau_0' & & \\
& & \ddots & \\
0 & & & \\
\end{pmatrix}.
$$

The matrix $A$ is symmetric. In order to ensure positive eigenvalues we apply the Gershgorin theorem. We have

$$
\tau_0' \geq 2 \quad \Rightarrow \tau_0 \geq \frac{2}{h} .
$$

From the above we conclude that using the second order accurate SBP operator, the numerical interface treatment (3.8) is stable for

$$
\tau_N = \frac{1}{2}, \quad \gamma_N = -\frac{1}{2}, \quad \tau_0 \geq \frac{2}{h}, \quad \tau_1 \geq 0 .
$$

**Fourth order accurate SBP operator** The Fourth order operator $D_x$ is

$$
S = \frac{1}{h} \begin{pmatrix}
-d_0 & d_1 & d_2 & -d_3 & d_4 & \cdots \\
\cdots & -d_4 & d_3 & -d_2 & -d_1 & d_0 \\
\end{pmatrix},
$$

$$
d_i \geq 0, \quad d_0 - d_1 - d_2 + d_3 - d_4 = 0 .
$$
Substituting $D_x$ in (3.12), we have

$$(Qw)_N = \frac{1}{h} \left[ -d_4 u_{N-4} + d_3 u_{N-3} - d_2 u_{N-2} - d_1 u_{N-1} + d_0 u_N + d_0 v_0 + d_1 v_1 + d_2 v_2 - d_3 v_3 + d_4 v_4 \right] - \tau_0 (u_N - v_0),$$  

(3.27)

and

$$(Qw)_{N+1} = -(Qw)_N.$$  

We set $\tau_0 = \frac{\tau'_0 - d_4}{h}$ and rearrange (3.27) to

$$(Qw)_N = -\frac{1}{h} (Aw)_N + \frac{1}{h} (Aw)_{N+1}$$  

(3.28)

$$(Qw)_{N+1} = \frac{1}{h} (Aw)_N - \frac{1}{h} (Aw)_{N+1}.$$  

(3.29)

where

$$(Aw)_N = d_4 u_{N-4} - (d_3 - d_4) u_{N-3} - (d_1 - d_0) u_{N-2} + d_0 u_{N-1} +$$  

$$+ (\tau'_0 - d_4) u_N + d_0 v_0 +$$  

$$- (d_1 - d_0) v_1 - (d_3 - d_4) v_2 + d_4 v_3,$$  

(3.30)

and

$$(Aw)_{N+1} = d_4 u_{N-3} - (d_3 - d_4) u_{N-2} - (d_1 - d_0) u_{N-1} + d_0 u_N +$$  

$$+ (\tau'_0 - d_4) v_0 + d_0 v_1 +$$  

$$- (d_1 - d_0) v_2 - (d_3 - d_4) v_3 + d_4 v_4,$$  

(3.31)

Note that one can easily reach (3.27) by substituting (3.30) and (3.31) in (3.28). The matrix $A$ is then

$$A = (a_{ij}) = \begin{cases} \tau'_0 - d_4 & i = j \\ d_0 & |i - j| = 1 \\ -d_1 + d_0 & |i - j| = 2 \\ -d_3 + d_4 & |i - j| = 3 \\ d_4 & |i - j| = 4 \\ 0 & \text{otherwise} \end{cases}$$  

(3.32)

Applying the Gershgorin theorem to ensure that $A$ is positive definite we have

$$a_{ii} = \tau'_0 - d_4 \geq 2 \sum_{j=1, j\neq i}^{n} |a_{ij}|$$  

$$\Rightarrow \tau'_0 \geq \frac{2}{h} \sum_{j=1, j\neq i}^{n} |a_{ij}|$$  

$$\Rightarrow \tau_0 \geq \frac{2}{h} (d_0 + |d_0 - d_1| + |d_4 - d_3| + d_4).$$  

(3.33)
We have a stable method if (3.33) holds. Replacing $d_i$ with the values from SBP operators used in this thesis we have

$$\tau_0 \geq \frac{5.3332}{h}. \quad (3.34)$$

**Sixth order accurate SBP operator** The sixth order operator $D_x$ is

$$S = \frac{1}{h} \begin{pmatrix} -d_0 & d_1 & -d_2 & -d_3 & -d_4 & d_5 & -d_6 & \cdots \\ \vdots & d_6 & -d_5 & d_4 & d_3 & d_2 & -d_1 & d_0 \end{pmatrix} \quad (3.35)$$

$$d_i > 0, \quad -d_0 + d_1 - d_2 - d_3 - d_4 + d_5 - d_6 = 0$$

Substituting $D_x$ in (3.12), we have

$$(Q\mathbf{w})_N = \frac{1}{h} \left[ d_6 \mathbf{u}_{N-6} - d_5 \mathbf{u}_{N-5} + d_4 \mathbf{u}_{N-4} + d_3 \mathbf{u}_{N-3} + d_2 \mathbf{u}_{N-2} + \right.$$\left.$$ -d_1 \mathbf{u}_{N-1} + d_0 \mathbf{u}_N + \\
- d_0 \mathbf{v}_0 + d_1 \mathbf{v}_1 - d_2 \mathbf{v}_2 - d_3 \mathbf{v}_3 - d_4 \mathbf{v}_4 + d_5 \mathbf{v}_5 - d_6 \mathbf{v}_6 \right] + \\
- \tau_0 (\mathbf{u}_N - \mathbf{v}_0),$$

and

$$(Q\mathbf{w})_{N+1} = -(Q\mathbf{w})_N.$$ We set $\tau_0 = \frac{\tau_0 - d_6}{h}$ and rearrange (3.36) to (3.28) where

$$(A\mathbf{w})_N = -d_0 \mathbf{u}_{N-6} + (-d_6 + d_5) \mathbf{u}_{N-5} + (-d_6 + d_5 - d_4) \mathbf{u}_{N-4} + \quad (3.37)$$

$$+(d_2 - d_1 + d_0) \mathbf{u}_{N-3} + (-d_1 + d_0) \mathbf{u}_{N-2} + d_0 \mathbf{u}_{N-1} + (\tau'_0 - d_6) \mathbf{u}_N + \\
+d_0 \mathbf{v}_0 + (-d_1 + d_0) \mathbf{v}_1 + (d_2 - d_1 + d_0) \mathbf{v}_2 + (-d_6 + d_5 - d_4) \mathbf{v}_3 + \\
+(-d_6 + d_5) \mathbf{v}_4 - d_6 \mathbf{v}_5,$$

and

$$(A\mathbf{w})_{N+1} = -d_6 \mathbf{u}_{N-5} + (-d_6 + d_5) \mathbf{u}_{N-4} + (-d_6 + d_5 - d_4) \mathbf{u}_{N-3} + \quad (3.38)$$

$$+(d_2 - d_1 + d_0) \mathbf{u}_{N-2} + (-d_1 + d_0) \mathbf{u}_{N-1} + d_0 \mathbf{u}_N + (\tau'_0 - d_6) \mathbf{v}_0 + \\
+d_0 \mathbf{v}_1 + (-d_1 + d_0) \mathbf{v}_2 + (d_2 - d_1 + d_0) \mathbf{v}_3 + (-d_6 + d_5 - d_4) \mathbf{v}_4 + \\
+(-d_6 + d_5) \mathbf{v}_5 - d_6 \mathbf{v}_6,$$

Note that one can easily reach (3.36) by substituting (3.37) and (3.38) in
The matrix $A$ is then

$$A = (a_{ij}) = \begin{cases} 
\tau'_0 - d_6 & i = j \\
d_0 & |i - j| = 1 \\
-d_1 + d_0 & |i - j| = 2 \\
d_2 - d_1 + d_0 & |i - j| = 3 \\
-d_4 + d_5 - d_6 & |i - j| = 4 \\
d_5 - d_6 & |i - j| = 5 \\
-d_6 & |i - j| = 6 \\
0 & \text{otherwise}
\end{cases}$$

Using the Gershgorin theorem we have

$$\tau'_0 - d_6 \geq 2(d_0 + |d_0 - d_1| + |d_2 - d_1 + d_0| + | - d_4 + d_5 - d_6| + |d_5 - d_6| + d_6)$$

$$\Rightarrow \tau_0 \geq \frac{2}{h}(d_0 + |d_0 - d_1| + |d_2 - d_1 + d_0| + | - d_4 + d_5 - d_6| + |d_5 - d_6| + d_6).$$

We have a stable 6th order accurate method if (3.40) holds. Replacing $d_i$ with the values from the SBP operators used in this thesis we have

$$\tau_0 \geq \frac{6.9363}{h}. \quad (3.41)$$

4 The Perfectly Matched Layer

In this section we will derive the PML for the 2D wave equation in a discontinuous media. We will derive corresponding modified material interface condition for the PML. We will also prove stability of the PML in homogeneous and discontinuous media.

Consider the wave equation in a discontinuous media

$$\frac{1}{c_1^2} u_{1tt} = u_{1xx} + u_{1yy}, \quad y \in \Omega_1 = (-\infty, 0), \quad x \in \mathbb{R}, \quad (4.1)$$

$$\frac{1}{c_2^2} u_{2tt} = u_{2xx} + u_{2yy}, \quad y \in \Omega_2 = (0, \infty), \quad x \in \mathbb{R}, \quad (4.2)$$

with $c_1 \neq c_2$ where the physical interface is placed at $y = 0$ and the conditions are

$$\begin{cases}
    u_1 = u_2 \\
    c_1^2 u_{1y} = c_2^2 u_{2y}.
\end{cases} \quad (4.3)$$

Assume that we are interested in computing the solution in the right half-plane $0 \leq x < \infty$. To absorb out-going waves, we introduce the PML in the left half-plane. The PML is derived by analytically continuing the equations
to the complex contour. We start by taking Fourier transformation in time, we have
\[
\begin{align*}
-\frac{\omega^2}{c_1^2} \hat{u}_1 &= \hat{u}_{1xx} + \hat{u}_{1yy}, & y \in \Omega_1, & x \in \mathbb{R}, \\
-\frac{\omega^2}{c_2^2} \hat{u}_2 &= \hat{u}_{2xx} + \hat{u}_{2yy}, & y \in \Omega_2, & x \in \mathbb{R}.
\end{align*}
\] (4.4) (4.5)

We analytically continue (4.4) and (4.5) on the complex contour,
\[
\tilde{x} = x + \frac{\Gamma(x)}{i \omega},
\] (4.6)

Here \( \Gamma(x) \) is a smooth, non-negative and increasing function. Changing the coordinates to \( \tilde{x} \) we have
\[
\begin{align*}
-\frac{\omega^2}{c_1^2} \hat{u}_1 &= \frac{1}{S_x} \left( \frac{1}{S_x} \hat{u}_{1x} \right) + \hat{u}_{1yy}, & y \in \Omega_1, \\
-\frac{\omega^2}{c_2^2} \hat{u}_2 &= \frac{1}{S_x} \left( \frac{1}{S_x} \hat{u}_{2x} \right) + \hat{u}_{2yy}, & y \in \Omega_2,
\end{align*}
\] (4.7) (4.8)

where
\[
S_x = 1 + \frac{\sigma(x)}{i \omega}, \quad \sigma(x) = \frac{d}{dx} \Gamma(x).
\] (4.9)

The smooth function \( \sigma(x) \) which is zero in the interior and positive in the PML is called the damping function. Note that
\[
\frac{1}{S_x} = 1 - \frac{1}{S_x i \omega} \iff 1 = \frac{1}{S_x} + \frac{\sigma(x)}{i \omega} \iff \frac{1}{S_x} = 1 - \frac{1}{S_x i \omega}.
\] (4.10)

Multiplying equations (4.7) and (4.8) by \( S_x \) and substituting (4.10) we have
\[
\begin{align*}
-\frac{\omega^2}{c_1^2} \hat{u}_1 &= \left( 1 - \frac{1}{S_x i \omega} \right) \hat{u}_{1x} + S_x \hat{u}_{1yy}, & y \in \Omega_1, \\
-\frac{\omega^2}{c_2^2} \hat{u}_2 &= \left( 1 - \frac{1}{S_x i \omega} \right) \hat{u}_{2x} + S_x \hat{u}_{2yy}, & y \in \Omega_2,
\end{align*}
\] (4.11) (4.12)

Note that in (4.11) and (4.12) the flux in the \( y \) direction changes to
\[
\hat{u}_{1y} \to S_x \hat{u}_{1y}, \quad \hat{u}_{2y} \to S_x \hat{u}_{2y}.
\] (4.13)

To localize in time we introduce two auxiliary variables \( \hat{v} = \frac{1}{S_x i \omega} \hat{u}_x \) and \( \hat{w} = \frac{\hat{u}_y}{i \omega} \) and apply inverse Fourier transform to (4.11) and (4.12). We have
\[
\begin{align*}
\frac{1}{c_1^2} \left( u_{1tt} + \sigma u_{1t} \right) &= u_{1xx} + u_{1yy} - (\sigma v_1)_t + \sigma w_1, & y \in \Omega_1, \\
v_{1t} &= u_{1x} - \sigma v_1, \quad w_{1t} = u_{1y}.
\end{align*}
\] (4.14)
and
\[
\begin{cases}
\frac{1}{c_2^2} (u_{2tt} + \sigma u_{2t}) = u_{2xx} + u_{2yy} - (\sigma v_2)_x + \sigma w_2, & y \in \Omega_2, \\
v_{2t} = u_{2x} - \sigma v_2, & w_{2t} = u_{2y}
\end{cases}
\] (4.15)

We note in passing that if \( \sigma(x) = 0 \) we recover the original systems (4.1) and (4.2). If \( \sigma(0) = 0 \), the PML (4.14) and (4.15) are perfectly matched to the wave equations (4.1) and (4.2). There are no reflections as waves pass into the PML. The PML damps the waves so that they become insignificant before they reach the outer boundaries.

### 4.1 Interface conditions

In constructing the PML we noted in (4.13) that the flux changes in \( y \) direction. To ensure numerical accuracy, physical interface conditions must be transformed to correspond to the PML. Note that the PML is applied to the x-derivatives. Thus the physical interface condition (4.3) is enough to ensure perfect matching for the continuous PML.

However, in numerical experiments (see section 6) using only (4.3) leads to larger numerical errors. In order to minimize numerical errors, we derive new transformed interface conditions by modifying (4.3).

Consider the physical interface conditions (4.3). We take the Fourier transformation in time. We have
\[
c_1^2 \hat{u}_{1y} = c_2^2 \hat{u}_{2y}.
\] (4.16)

We multiply (4.16) by \( S_x \). Note that this corresponds to the change of flux in (4.13). We have
\[
c_1^2 \hat{u}_{1y} + c_1^2 \sigma(x) \hat{u}_{1y} = c_2^2 \hat{u}_{2y} + c_2^2 \sigma(x) \hat{u}_{2y}.
\] (4.17)

Introducing \( w_j = \frac{\hat{u}_j}{i\omega}, j \in \{1, 2\} \) and applying Inverse Fourier Transform, we have
\[
\left\{ \begin{array}{l}
u_1 = u_2 \\
c_1^2 (u_{1y} + \sigma(x) w_1) = c_2^2 (u_{2y} + \sigma(x) w_2).
\end{array} \right.
\] (4.18)

Equations (4.18) are the transformed interface conditions for the PML. Note that if \( \sigma(x) = 0 \) we recover the physical interface conditions (4.3).

In the continuous settings, from the interface conditions we have
\[
c_1^2 u_{1y} = c_2^2 u_{2y},
\]
integrating both sides over time and multiplying by $\sigma(x)$ we have

$$
\sigma(x)c_1^2 \int_0^t u_{1y} \, dt = \sigma(x)c_2^2 \int_0^t u_{2y} \, dt.
$$

(4.19)

We assume $w_1(0, x) = 0, w_2(0, x) = 0$. We can replace $\int_0^t u_{1y} \, dt$ and $\int_0^t u_{2y} \, dt$ with their equivalent in (4.14) and (4.15) we have

$$
c_1^2 \sigma(x)w_1 = c_2^2 \sigma(x)w_2.
$$

Adding the equality above to (4.3) we reach (4.18). Hence, (4.18) and (4.3) are mathematically equivalent.

4.2 Stability

In this section we will prove the stability of the PML for the homogeneous and discontinuous media.

4.2.1 Stability for homogeneous media

Consider the PML

$$
\frac{1}{c^2} u_{tt} + \sigma c^2 u_t = u_{xx} + u_{yy} - (\sigma v)_x + \sigma w_y
$$

(4.20)

$$
v_t = u_x - \sigma v
$$

(4.21)

$$
w_t = u_y,
$$

(4.22)

on a homogeneous media. We consider the damping profile $\sigma$ to be constant, we seek solutions of the form

$$
\begin{pmatrix}
u \\
v \\
w
\end{pmatrix} = e^{\omega t + ik_x x + ik_y y}
\begin{pmatrix}
u_0 \\
v_0 \\
w_0
\end{pmatrix}.
$$

(4.23)

Inserting (4.23) in the PML we have

$$
\begin{pmatrix}
\omega^2 + \sigma \omega + k_x^2 + k_y^2 & -i\sigma k_x & i\sigma k_y \\
 i k_x & \omega + \sigma & 0 \\
 i k_y & 0 & \omega
\end{pmatrix}
\begin{pmatrix}
u \\
v \\
w
\end{pmatrix} = 0.
$$

(4.24)

To ensure non-trivial solutions, the coefficient matrix must be singular. We have

$$
\omega^4 + 2\sigma \omega^3 + (k_x^2 + k_y^2 + \sigma^2) \omega^2 + 2\sigma k_y^2 \omega + \sigma^2 k_y^2 = 0.
$$

(4.25)

Note that instability occurs if $\text{Re}(\omega) > 0$. We introduce normalized variables

$$
\lambda = \frac{\omega}{|k|}, \quad \epsilon = \frac{\sigma}{|k|}, \quad k_1 = \frac{k_x}{|k|}, \quad k_2 = \frac{k_y}{|k|}, \quad k = \sqrt{k_x^2 + k_y^2}.
$$

(4.26)
By inserting (4.26) in (4.25) we have
\[ \lambda^4 + 2\epsilon\lambda^3 + (1 + \epsilon^2)\lambda^2 + 2\epsilon k_2^2\lambda + \epsilon^2 k_2^2 = 0. \]  
(4.27)
We apply perturbation analysis to \( \lambda \). Consider
\[ \lambda = \lambda_0 + \epsilon\lambda_1, \]  
(4.28)
where \( \lambda \) is a complex number. If \( \epsilon = 0 \) we have
\[ \lambda_0 \in \{0, \pm i\}. \]  
(4.29)
We apply perturbation analysis to (4.27) and we omit the higher order of \( \epsilon \). We have
\[ (\lambda_0^4 + \lambda_0^2) + (4\lambda_1\lambda_0^3 + 2\lambda_0^3 + 2\lambda_1\lambda_0 + 2\lambda_0 k_2^2)\epsilon = 0. \]  
(4.30)
We solve (4.30) to find
\[ \lambda_1 = -1 + k_2^2 = -k_1^2 < 0, \quad \lambda_0 = \pm i \]  
(4.31)
The PML is stable since \( \Re \lambda_1 \leq 0 \).

4.2.2 Stability for discontinuous media
Consider (4.14) and (4.15) with constant wave speeds \( c_1 \neq c_2 \) and constant damping function \( \sigma \). We seek solutions of the form
\[ \begin{pmatrix} u_j \\ v_j \\ w_j \end{pmatrix} = e^{st+ik_x x} \begin{pmatrix} \hat{u}_j(y) \\ \hat{v}_j(y) \\ \hat{w}_j(y) \end{pmatrix}, \quad j = 1, 2 \]  
(4.32)
Note that if there is a non-trivial solution for \( \Re s > 0 \), the system (4.14) and (4.15) allow growing modes, while if \( \Re s \leq 0 \) for all solutions, there are no growing modes. Inserting (4.32) in (4.14) and (4.15) we have
\[ s^2 \hat{u}_j + \sigma s \hat{u}_j = -c_j^2 k_x^2 \hat{u}_j + c_j^2 \hat{u}_{jyy} - i\sigma k_x c_j^2 \hat{v}_j + \sigma c_j^2 \hat{w}_j \]  
(4.33)
\[ s \hat{v}_j = ik_x \hat{u}_j - \sigma \hat{v}_j \]  
(4.34)
\[ s \hat{w}_j = \hat{u}_j \]  
(4.35)
substituting (4.34) and (4.35) in (4.33) we have
\[ s^2 \hat{u}_j + \sigma s \hat{u}_j = -c_j^2 k_x^2 \hat{u}_j + c_j^2 \hat{u}_{jyy} + \frac{\sigma k_x^2 c_j^2}{s + \sigma} \hat{u}_j + \frac{\sigma c_j^2}{s} \hat{u}_{jyy} \]  
We introduce \( S_x = (1 + \frac{\alpha}{s}) \) and \( \tilde{k}_x = \frac{\tilde{k}_x}{s_x} \), we have system of ODEs
\[ \frac{s^2}{c_j^2} \hat{u}_j = \hat{u}_{jyy} - \tilde{k}_x^2 \hat{u}_j, \quad j = 1, 2 \]  
(4.36)
Replacing \( u_j(y) = \psi e^{\kappa_j y} \) we have

\[
\frac{s^2}{c_j^2} = \kappa_j^2 - \tilde{k}_x^2 \iff \kappa_j^2 = \frac{s^2}{c_j^2} + \tilde{k}_x^2
\]

\[
\iff \kappa_j = \pm \sqrt{\frac{s^2}{c_j^2} + \tilde{k}_x^2}.
\]

(4.37)

The solutions to the ODEs (4.36) are

\[
\hat{u}_1(y) = \psi_1 e^{\kappa_1 y}
\]

(4.38)

\[
\hat{u}_2(y) = \psi_2 e^{-\kappa_2 y}
\]

(4.39)

Applying the interface conditions to (4.38) and (4.39) we have

\[
\begin{pmatrix} 1 & -1 \\ c_1^2 \kappa_1 & c_2^2 \kappa_2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\]

(4.40)

To ensure non-trivial solutions, the coefficient matrix should be singular. We have

\[
c_1^2 \kappa_1 + c_2^2 \kappa_2 = 0
\]

\Rightarrow \left( c_1^2 \kappa_1 \right)^2 - \left( c_2^2 \kappa_2 \right)^2 = 0

\Rightarrow c_1^2 \left( \frac{s^2}{c_1^2} + \tilde{k}_x^2 \right) - c_2^2 \left( \frac{s^2}{c_2^2} + \tilde{k}_x^2 \right) = 0

\Rightarrow (c_1^2 - c_2^2) \left( s^2 + (c_1^2 + c_2^2) \tilde{k}_x^2 \right) = 0

\Rightarrow s^2 + (c_1^2 + c_2^2) \tilde{k}_x^2 = 0
\]

(4.41)

Replacing \( \tilde{k}_x \) and \( S_x \) in (4.41), we have

\[
s^2 \left( 1 + \frac{\sigma}{s} \right)^2 + (c_1^2 + c_2^2) \tilde{k}_x^2 = 0
\]

\Rightarrow (s + \sigma)^2 + (c_1^2 + c_2^2) \tilde{k}_x^2 = 0

\Rightarrow s = -\sigma - i \sqrt{(c_1^2 + c_2^2) k_x}

\Rightarrow Re(s) < 0.
\]

(4.42)

Hence the PML is stable.

5 Discrete approximation of the PML in a discontinuous media

In this section we will derive the semi-discrete approximation of the PML using SBP operators. The boundary and the physical interface condition will
be imposed weakly using SAT method. The semi-discrete wave equation will be approximated in time using the conservative time-stepping scheme [5], while the semi-discrete auxiliary differential equations will be discretized in time using the Crank-Nicolson scheme.

5.1 Semi-discrete problem

To begin, we define Kronecker products.

**Definition 2 (Kronecker products).** Let $A$ be an $m$-by-$n$ matrix and $B$ be a $p$-by-$q$ matrix. Then the Kronecker product of $A$ and $B$, is the $(m.p)$-by-$(n.q)$ matrix

$$ A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1}B & a_{n2}B & \cdots & a_{nm}B \end{pmatrix} $$

The following properties hold for Kronecker products

- Assume that the products $AC$ and $BD$ are well defined then $(A \otimes B) \cdot (C \otimes D) = (A \cdot C) \otimes (B \cdot D)$.
- If $A$ and $B$ are invertible, then $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$.
- $(A \otimes B)^T = A^T \otimes B^T$.

Consider the PML (4.14) and (4.15) in a discontinuous media, the semi-discrete approximation of the equations are

$$ C \frac{d^2 u}{dt^2} + \sigma \frac{du}{dt} = D_{xx}u + D_{yy}u - D_x(\sigma v) + D_y(\sigma w) - \tau_N H^{-1} \tilde{B}_n(D_y u + \sigma w) - \gamma_N H^{-1} D_y^T \tilde{B}_n^T u $$

$$ \frac{dv}{dt} = D_y u - \sigma v $$

$$ \frac{dw}{dt} = D_y u. $$

Here $u, v, w, C, \sigma, D_{xx}, D_{yy}, D_y, \tilde{B}_n, \hat{B}_n$ and $D_x$ are

$$ u = [u_1, u_2]^T, \quad v = [v_1, v_2]^T, \quad w = [w_1, w_2]^T, $$

$$ \tilde{B}_n = I_2 \otimes I_m \otimes \tilde{B}, \quad \hat{B}_n = I_2 \otimes I_m \otimes \hat{B}, \quad D_x = I_2 \otimes D_1 \otimes I_n, $$

$$ D_{xx} = I_2 \otimes D_2 \otimes I_n, \quad D_y = I_2 \otimes I_m \otimes D_1, \quad D_{yy} = I_2 \otimes I_m \otimes D_2, $$

$$ C = \begin{pmatrix} \frac{1}{\epsilon_1^2} I & 0 \\ 0 & \frac{1}{\epsilon_2^2} I \end{pmatrix}. $$

25
Note that $0$ is a zero matrix and $I_2, I_m, I_n$ are identity matrices of size 2, $m$ and $n$. The matrices $D_1$ and $D_2$ are the SBP operators approximating $(\partial / \partial x), (\partial^2 / \partial x^2)$. The matrices $\tilde{B}$ and $\tilde{B}$ are the interface operators defined in (3.9) and (3.10). In (5.1) the first line of the equation is the semi-discrete approximation of (4.14) and (4.15). In the second line, the first term is discrete imposition of the interface condition $(\partial / \partial x)u_1 + \sigma w_1 = (\partial / \partial x)u_2 + \sigma w_2$. The rest of the RHS impose $u_1 = u_2$. Equations (5.2) and (5.3) are the semi-discrete auxiliary differential equations.

5.2 Fully discrete approximation

We begin by defining finite difference operators in time domain. Let $\Delta t$ denote the time step and $t_n = n\Delta t$. We denote $u^n \approx u(t_n)$. The finite difference operators (with respect to time) are denoted

\begin{align*}
D_{tt}^n u^n &= \frac{1}{\Delta t^2} (u^{n+1} - 2u^n + u^{n-1}), \\
S^t u^n &= u^{n+1}, \\
D_t^0 u^n &= \frac{1}{2\Delta t} (u^{n+1} - u^{n-1}).
\end{align*}

The time integration uses the compact time-stepping scheme [5], for the physical variable $u$ and the Crank-Nicolson scheme for the auxiliary variables $v, w$. A second order accurate time-marching scheme is

\begin{align*}
CD_{tt}^n u^n + \sigma D_t^0 u^n &= D_2 u^n - D_x (\sigma v^n) + \tilde{D} w^n, \\
D_t^v v^n &= \frac{1}{2} (I + S^t)(D_x u^n - \sigma v^n), \\
D_t^w w^n &= \frac{1}{2} (I + S^t)(D_y u^n).
\end{align*}

Here $D_2, \tilde{D}$ are

\begin{align*}
D_2 &= D_{xx} + D_{yy} - \tau_n H^{-1} \tilde{B}_n D_y - \gamma_N H^{-1} D_y ^T \tilde{B}^T - \tau_0 H^{-1} \tilde{B}_n, \\
\tilde{D} &= \sigma D_y - \kappa \tau_N \sigma H^{-1} \tilde{B}_n.
\end{align*}

Note that if $\kappa = 0$ we have the physical interface conditions (4.3) and if $\kappa = 1$ the interface treatment corresponds to the modified interface condition (4.18). We define

\begin{equation}
D_4 = D_2 + \frac{\Delta t^2}{12} D_2^2.
\end{equation}

The fourth order time stepping scheme is

\begin{align*}
CD_{tt}^n u^n + \sigma D_t^0 u^n &= D_4 u^n - D_x (\sigma v^n) + \tilde{D} w^n, \\
D_t^v v^n &= \frac{1}{2} (I + S^t)(D_x u^n - \sigma v^n), \\
D_t^w w^n &= \frac{1}{2} (I + S^t)(D_y u^n).
\end{align*}
Note that in (5.16), the interior is fourth order accurate in time and the absorbing layer uses second order accurate time stepping. Also the auxiliary variables $v,w$ are approximated using second order accurate scheme in time.

Let $\lambda_j$ denote the eigenvalues of $D$. If $\sigma = 0$, the second order time-stepping (5.10), (5.11), (5.12) is stable if

$$\Delta t < \frac{2}{\sqrt{\max |\lambda_j|}}.$$  (5.19)

The fourth order scheme (5.16), (5.17), (5.18) is stable if

$$\Delta t < \frac{2\sqrt{3}}{\sqrt{\max |\lambda_j|}}.$$  (5.20)

The proof of stability of the interior scheme is studied in [5]. We note that the spatial accuracy of the scheme is the same as the order of accuracy of the interior scheme. For second order accurate SBP operators, we use the second order accurate time stepping scheme. For higher order accurate SBP operators the fourth order accurate time stepping scheme is used.

6  Numerical experiments

In this section we will present numerical experiments. We will begin by studying the convergence and accuracy of the interface treatment without the PML. We will proceed to investigate numerically the accuracy and convergence of the PML. We would like to understand the influence of the transformed interface conditions (4.18) compared to the physical interface conditions (4.3). We will start with a wide PML and a fixed damping profile to see the effects of numerical reflections from the interface. Next the overall reflection error is evaluated using a short width PML and a damping coefficient that depends on the spatial step size. Lastly, we will investigate the effects of having multiple layers by adding more interfaces.

To begin, we set our computational domain $(x, y) \in [-1,1] \times [-2,2]$. We add the absorbing layer in $x$ direction $(x, y) \in [-1,1+\delta] \times [-2,2]$. The computational setups are shown in figure 1.

First we consider a homogeneous media with a physical artificial interface at $y = 0$. In the experiments if the domain consists of four layers, the physical interfaces are placed at $y = \{0, \pm 1\}$. We discretize the domain with uniform spatial steps $\Delta x = \Delta y = h$ in both $x$ and $y$-directions. Consider initial data

$$u(x, y, 0) = e^{-\frac{(x-0.75)^2+(y-0.5)^2}{0.01}}, \quad \frac{\partial u}{\partial t}(x, y, 0) = 0.$$  (6.1)
The boundary conditions are
\[
\begin{align*}
\frac{\partial u}{\partial x}(x, -2, t) &= 0, & \frac{\partial u}{\partial x}(x, 2, t) &= 0, \\
\frac{\partial u}{\partial y}(-1, y, t) &= 0, & \frac{\partial u}{\partial x}(1 + \delta, y, t) &= 0.
\end{align*}
\]
(6.2) \hspace{2cm} (6.3)

The damping function is a monomial of degree three
\[
\sigma(x) = \begin{cases} 
0, & x \leq 1, \\
d_0 \left(\frac{x-1}{\delta}\right)^3, & x \geq 1, \end{cases} \quad d_0 > 0.
\]
(6.4)

When a wide PML is used we set \(d_0 = 400\) and for small width PML, the damping coefficient is
\[
d_0 = \frac{4}{2\delta} \log \left(\frac{1}{(C_0 h)^p}\right),
\]
(6.5)
where \(p = 2, 4\) for second and fourth order accurate scheme respectively and \(C_0 = 10^{-4}\) is empirically determined.

In numerical computations, when the PML is used in a discontinuous media, 3 different types of errors are introduced: The discretization error, the modeling error and the numerical reflection. The discretization error is the error caused by using any numerical method (for example by using SBP operators to approximate derivatives). The modeling error is introduced by using a finite width PML. The numerical reflection error is the non-physical reflections introduced into the physical domain and caused by discretizing the PML. The discretization error and numerical reflection should vanish as the mesh-size approaches zero. The modeling error decreases when the magnitude of the damping coefficient increases or the PML width increases.
6.1 Interface treatment without PML

Consider a homogeneous media and scale time such that the wave speed is $c = 1$. We introduce an artificial physical interface at $y = 0$. We set the penalty terms for the interface treatment $\tau_0 = 6/h, \tau_N = 0.5, \gamma_N = -0.5$ and compute the solution until $t = 5$ with the time step $\Delta t = 0.1h$. The error is computed by comparing the solution obtained with the solution of the wave equation in a single domain. The results are presented in table 1. We can see that second order accurate scheme is exact, that is, the error is as small as machine precision. Our second order interface treatment is completely transparent. As the grid is refined, the error in fourth order scheme approaches zero with convergence rate of higher than four.

<table>
<thead>
<tr>
<th>Mesh size (h)</th>
<th>2-nd order</th>
<th>4-th order</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Rate</td>
<td>Error</td>
</tr>
<tr>
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<td>-</td>
<td>$2.474 \times 10^{-13}$</td>
</tr>
<tr>
<td>0.02</td>
<td>0.8067</td>
<td>$1.415 \times 10^{-14}$</td>
</tr>
<tr>
<td>0.01</td>
<td>1.471</td>
<td>$3.92 \times 10^{-14}$</td>
</tr>
</tbody>
</table>

Table 1: Interface treatment for homogeneous media with artificial interface

Figure 2 shows the error as a function of time. We see that the error in second order accurate scheme rises as the time pass but in fourth order accurate scheme the errors are level in time.

6.2 Interface treatment with wide PML

In this part a homogeneous medium with an artificial interface at $y = 0$ is considered. The same settings as in section 6.1 are used for this experiment. We add a PML with width $\delta = 6$ and constant damping coefficient of $d_0 =$
Figure 3: The dynamics of the pressure field $|u|$ inside a waveguide in a homogeneous media with speed $c = 1$ and an artificial physical interface at $y = 0$ bounded by Neumann boundary conditions at $x = -1, y = \pm 2$ and the waveguide is truncated at $x = 1$ with the PML of width $\delta = 0.5$. The snapshots are given at $t = 0.4, 0.8, 1.4, 1.8$.

The error and convergence rate is calculated for $\kappa = 0$ and also for $\kappa = 1$. The error at $t = 5$ and the convergence rate are shown in tables 4a and 5a. We see in table 4a that when the original interface conditions (3.5) are used ($\kappa = 0$) the method converges but the convergence rate is not optimal. The second order accurate scheme is only first order accurate and the fourth order accurate scheme is less than third order accurate. Table 5a shows that when the transformed interface conditions (4.18) are used we recover the optimal convergence rate and the error is smaller in magnitude. Here the second order accurate scheme has the convergence rate of 2 and the fourth order accurate scheme has the convergence rate of more than 4.

Figure 4 shows the error as a function of time when $\kappa = 0$. We see that errors are small until the waves penetrate the PML.

When $\kappa = 1$, from figure 5 we see that the errors start growing when the waves enter the PML but the growth level off as time passes.
Here we consider the wave equation in a homogeneous media with an artificial interface at \( y = 0 \). The settings are the same as section 6.2. The PML width is changed to \( \delta = 0.5 \) and the damping coefficient depends on the spatial step size \( h \)

\[
d_0 = \frac{(n + 1)C}{28} \log\left(\frac{1}{C_0 h}\right)^p, \quad C = \max\text{(speed)},
\]

where \( p = 2, 4 \) for second and fourth order accurate scheme respectively and \( C_0 = 10^{-4} \) is empirically determined. The solution is computed until time \( t = 5 \). The results are shown in tables 2 and 3. We see that the modeling errors are larger compared to results from section 6.2 (tables 4a and 5a) since the PML has smaller width which causes the modeling error to have larger magnitude. When \( \kappa = 0 \) we see in table 2 that the convergence rate is
Figure 6: The dynamics of the pressure field $|u|$ inside a waveguide in a discontinuous media with speeds $c_1 = 1$ if $y \leq 0$ and $c_2 = 2$ if $y \geq 0$ and a physical interface at $y = 0$ bounded by Neumann boundary conditions at $x = -1, y \pm 2$ and the waveguide is truncated at $x = 1$ with the PML of width $\delta = 0.5$. The snapshots are given at $t = 0.4, 0.8, 1.4, 1.8$.

not optimal. The second order accurate scheme first order accurate and the fourth order accurate scheme is less than third order accurate. Changing $\kappa = 1$, the optimal convergence rate is recovered. The second order scheme is almost second order accurate and the fourth order scheme is fourth order accurate.

<table>
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</thead>
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<td>Error</td>
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<tr>
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<td>1016</td>
<td>1.358 x 10^{-02}</td>
</tr>
<tr>
<td>0.02</td>
<td>1015</td>
<td>6.716 x 10^{-03}</td>
</tr>
<tr>
<td>0.01</td>
<td>1015</td>
<td>6.716 x 10^{-03}</td>
</tr>
</tbody>
</table>

Table 2: Thin PML with width 0.5, an artificial interface at $y = 0$ and $\kappa = 0$
Table 3: Thin PML with width 0.5, an artificial interface at $y = 0$ and $\kappa = 1$

<table>
<thead>
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<th>Mesh size (h)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Rate</td>
<td>Error</td>
</tr>
<tr>
<td>0.04</td>
<td>–</td>
<td>$1.921 \times 10^{-02}$</td>
</tr>
<tr>
<td>0.02</td>
<td>1.564</td>
<td>$6.497 \times 10^{-03}$</td>
</tr>
<tr>
<td>0.01</td>
<td>1.744</td>
<td>$1.939 \times 10^{-03}$</td>
</tr>
</tbody>
</table>

Figure 7: Interface treatment for a homogeneous media with artificial interface, thin PML and $\kappa = 0$

Figures 7 and 8 shows the error as a function of time. We see that errors are very small initially. As the waves penetrate the PML, the errors oscillates and grow in time. When $\kappa = 1$ the oscillations in the error are smaller compared to $\kappa = 0$.

Figure 8: Interface treatment for a homogeneous media with artificial interface, thin PML and $\kappa = 1$
6.4 Effects of multiple interfaces

In this section, the effects of multiple transformed interfaces on the accuracy and convergence rate are studied. The accuracy of the PML for $\kappa = 0$ and $\kappa = 1$ are compared. A wide PML $\delta = 5$ is considered with a constant damping coefficient $d_0 = 400$. The penalty term is $\tau_0 = 5$. Firstly, we consider two layers with speeds $c_1, c_2 \in \{1, 2, 4\}$ and a material interface at $y = 0$. We compute the solution for each pair of $c_1, c_2$ until time $t = 5$. Next we add two more material interfaces at $y = -1, y = 1$ to investigate the effects of multiple layers.

6.4.1 Artificial interfaces

We will investigate $\kappa = 0$ and $\kappa = 1$ separately. Consider a homogeneous media with the wave speed $c = 1$ and $\kappa = 0$. We first add an artificial material interface at $y = 0$ and compute the solution until $t = 5$. Next, two more artificial material interfaces are added at $y = -1, y = 1$ and the solution is computed until time $t = 5$. Results are shown in table 4. We see that when additional interfaces are introduced, the error grows and the convergence rate reduces. Note that the convergence rate is also not optimal. The second order accurate scheme is first order accurate and the fourth order accurate scheme has less than third order accuracy.

<table>
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</thead>
<tbody>
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<td>Rate</td>
<td>Error</td>
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<tr>
<td>0.01</td>
<td>1.039</td>
<td>$1.412 \times 10^{-04}$</td>
</tr>
</tbody>
</table>

(a) Wave speeds $(1, 1)$ and an artificial material interface at $y = 0$

<table>
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<th>Mesh size (h)</th>
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<th>4-th order</th>
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</thead>
<tbody>
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<td>Rate</td>
<td>Error</td>
</tr>
<tr>
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<td>$8.039 \times 10^{-04}$</td>
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<td>1.071</td>
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<td>1.031</td>
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</tr>
</tbody>
</table>

(b) Wave speeds $(1, 1, 1)$ and artificial material interfaces at $y = \{0, \pm 1\}$

Table 4: PML error and convergence rate for homogeneous media and $\kappa = 0$

Next, we set $\kappa = 1$ and compute the solutions. Table 5 shows the error and convergence rate of the solution. We see that adding additional interfaces to the domain have no effect on the convergence rate and the change in the errors are significantly small. We also recover the optimal convergence rate for the numerical method. The second order accurate scheme is second
order accurate and the fourth order accurate scheme is more than fourth order accurate.

<table>
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<th>4-th order</th>
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<td>0.02</td>
<td>2.008</td>
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</tr>
<tr>
<td>0.01</td>
<td>2.006</td>
<td>9.738 × 10^{-06}</td>
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(a) Wave speeds (1, 1) and an artificial material interface at y = 0

<table>
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</tr>
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<td>2.000</td>
<td>9.696 × 10^{-06}</td>
</tr>
</tbody>
</table>

(b) Wave speeds (1, 1, 1) and artificial material Interfaces at y = {0, ±1}

Table 5: PML error and convergence rate for homogeneous media and κ = 1

6.4.2 Discontinuous interfaces
Consider a discontinuous media with a material interface at y = 0. We set κ = 0 and compute the solution for the wave speeds c_1 = 1, c_2 = 2 and c_1 = 1, c_2 = 4, respectively. The results are presented in tables 6 and 7. We see that when the physical interface conditions (4.3) (κ = 0) is used, the numerical reflections grow as we add more interfaces. The convergence rate is also less than the optimal convergence rate.

<table>
<thead>
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<th>Mesh size (h)</th>
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<th>4-th order</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Rate</td>
<td>Error</td>
</tr>
<tr>
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<td>-</td>
<td>8.51 × 10^{-04}</td>
</tr>
<tr>
<td>0.02</td>
<td>1.077</td>
<td>4.034 × 10^{-04}</td>
</tr>
<tr>
<td>0.01</td>
<td>1.038</td>
<td>1.965 × 10^{-04}</td>
</tr>
</tbody>
</table>

(a) Wave speeds (1, 2) and an interface at y = 0

<table>
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<th>Mesh size (h)</th>
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<th>4-th order</th>
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<tr>
<td></td>
<td>Rate</td>
<td>Error</td>
</tr>
<tr>
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<td>-</td>
<td>1.312 × 10^{-03}</td>
</tr>
<tr>
<td>0.02</td>
<td>1.037</td>
<td>6.396 × 10^{-04}</td>
</tr>
<tr>
<td>0.01</td>
<td>1.021</td>
<td>3.153 × 10^{-04}</td>
</tr>
</tbody>
</table>

(b) Wave speeds (1, 1, 2) and interfaces at y = {0, ±1}

Table 6: Final error and convergence rate for discontinuous media with κ = 0
Next we set $\kappa = 1$ and compute the solutions. Results are shown in tables 8 and 9. We see that there are no changes in the convergence rate and the numerical errors are almost the same when the transformed interface condition (4.18) ($\kappa = 1$) is used. The optimal convergence rate is recovered.
Table 9: Final error and convergence rate for discontinuous media with $\kappa = 1$

### 6.5 Further development - 3D implementation

A C++ framework is being developed for numerical simulation of acoustic waves in three space dimensions. The analysis presented above can be straightforwardly extended to 3D.

Maintaining a balance between usefulness and performance of the code is one of the goals of this package. It is structured so that arbitrary number of layers can be introduced into the domain. Options to add force function and initial data as well as ways to use the solution in each time step or at the finale time is available. Figure 9 shows a simulation made using the 3D code. The domain consist of four layers with different speeds and the PML is place in the $y$-direction.

### 7 Conclusion

We present in this thesis applications of the perfectly matched layer (PML) in a discontinuous media. We consider the scalar wave equation in a discontinuous media. Using the energy method we derived stable interface conditions at the material interface. We used the SBP-SAT scheme to derive the semi-discrete approximation. Using the energy method we obtain sharp estimates for the penalty terms, thus proving the stability of the semi-discrete approximation. We derive the PML in a discontinuous media. We derived transformed interface conditions for the PML and prove stability using the modal ansatz.
Numerical experiments showed that using the proposed estimates for the penalty parameters, we have a stable and accurate discrete approximation for the wave equation. We also showed in our experiments that when the modified interface conditions are used in the discrete approximation of the PML, optimal accuracy is obtained and numerical reflections are smaller. We point out that the improvement to the accuracy of the scheme is also efficient since there is no overhead on the computations and no additional memory is needed.

References


