INTRODUCTION OF THE DEBYE MEDIA TO THE FILTERED FINITE-DIFFERENCE TIME-DOMAIN METHOD WITH COMPLEX-FREQUENCY-SHIFTED PERFECTLY MATCHED LAYER ABSORBING BOUNDARY CONDITIONS

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Abstract

The finite-difference time-domain (FDTD) method is one of most widely used computational electromagnetics (CEM) methods to solve the Maxwell’s equations for modern engineering problems. In biomedical applications, like the microwave imaging for early disease detection and treatment, the human tissues are considered as lossy and dispersive materials. The most popular model to describe the material properties of human body is the Debye model.

In order to simulate the computational domain as an open region for biomedical applications, the complex-frequency-shifted perfectly matched layers (CFS-PML) are applied to absorb the outgoing waves. The CFS-PML is highly efficient at absorbing the evanescent or very low frequency waves. This thesis investigates the stability of the CFS-PML and presents some conditions to determine the parameters for the one dimensional and two dimensional CFS-PML.

The advantages of the FDTD method are the simplicity of implementation and the capability for various applications. However the Courant-Friedrichs-Lewy (CFL) condition limits the temporal size for stable FDTD computations. Due to the CFL condition, the computational efficiency of the FDTD method is constrained by the fine spatial-temporal sampling, especially in the simulations with the electrically small objects or dispersive materials. Instead of modifying the explicit time updating equations and the leapfrog integration of the conventional FDTD method, the spatial filtered FDTD method extends the CFL limit by filtering out the unstable components in the spatial frequency domain. This thesis implements filtered FDTD method with CFS-PML and one-pole Debye medium, then introduces a guidance to optimize the spatial filter for improving the computational speed with desired accuracy.
Declaration

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Chapter 1

Introduction

Since 1940s, based on the evolution of the computer technology, the computational electromagnetics (CEM) methods have been widely used to study the communication systems, bio-electromagnetics and other subjects that involve the electromagnetic waves [1]. The CEM methods can be classified into two categories, the frequency domain methods and time domain methods. The frequency domain methods include the finite element method (FEM) [2][3], the fast multipole method (FMM) [4], the method of moments (MoM) [5][6] and so on. As one of the time domain methods, the finite-difference time-domain (FDTD) method is famous for its precise geometry structure and straightforward algorithm [7][8]. All these methods are developed for solving the electromagnetic problems in different circumstances.

1.1 Motivation

In 1966, Kane S. Yee published the original paper of the FDTD method [8]. Sampling the electromagnetic field components in both time and space, the Yee’s algorithm discretizes the Maxwell’s curl equations by using the central difference approximation, and solves these equations at each time step to update the electromagnetic field components. The solution of the FDTD method is second order accurate. As a time domain technique, the FDTD method is adaptable for various electromagnetic applications over a wide bandwidth.
1.2 Challenges

The major challenges of the FDTD method are to absorb the traveling waves at the boundary, to model the frequency dependent (FD) materials, to minimize the numerical dispersion and to extend the numerical stability [9][10].

The studies of the boundary conditions and dispersive materials improve the capability of the FDTD method to deal with practical problems like the biomedical therapies or early disease detections. In this thesis, the dispersive materials are simulated by the one-pole Debye model and the outgoing waves are attenuated by complex-frequency-shifted perfectly matched layers (CFS-PML) absorbing boundary conditions (ABC) [11][12].

The numerical dispersion affects the accuracy of the FDTD method. To guarantee the accuracy, the spatial size should be shorter than one tenth of the minimum excited wavelength [7]. For stable computations, the upper limit of the temporal size is constrained by the Courant–Friedrichs–Lewy (CFL) condition. As a result, the high temporal and spatial resolution reduce the computational efficiency and increase the memory cost for the FDTD method. To increase the computation speed, the filtered FDTD method extends the CFL limit conditionally by filtering out the unstable components in the high spatial frequencies [13].

1.3 Aim and Objectives

The aim of this research is to accelerate the computation speed of the FDTD method for biomedical applications. Thus the first objective of this thesis is introducing the one-pole Debye media to the filtered FDTD method with CFS-PML ABC. The filtered FD-FDTD method with CFS-PML is studied based on two points, the stability and accuracy. The stability of the spatial filtering approach is governed by a filtering wavenumber based on the revised CFL condition, which is derived from the lossless materials. Therefore the second objective of this thesis is to derive the revised stability condition for the spatial filtering approach with CFS-PML. The choice of the filtering wavenumber depends on the accuracy. However, in the previous publications like [13] and [14], the filtering wavenumber is mainly decided by experiences. For determining the filtering wavenumber, the third objective of this thesis is to investigate the key aspects that affect the accuracy of the filtered FD-FDTD method with CFS-PML.
1.4 Outline

This thesis consists of 7 chapters.

Chapter 2 reviews the background of the FDTD method with one-pole Debye model and CFS-PML. The mathematical formulations for the conventional FDTD method, the auxiliary differential equation (ADE) scheme for the Debye model and the convolutional PML with CFS stretching coefficient are presented.

The numerical dispersion, stability and phase velocity of the convention FDTD method are shown in Chapter 3. However, it is a challenge to derive the numerical stability for the FDTD method with CFS-PML ABC, since the numerical wavenumber in the CFS-PML computation is a complex number. This thesis derives the numerical dispersion relation of the CFS-PML, then presents some conditions to determine the temporal size for the CFS-PML.

Chapter 4 shows the basic idea of the spatial filtering approach and presents the revised CFL conditions for the filtered FDTD method. The revised stability of the filtered FDTD method with CFS-PML ABC is investigated based on the numerical dispersion relation of the CFS-PML. The last section of the chapter shows the procedures of the spatial filtering approach.

Chapter 5 presents the numerical experiments of the spatial filtering approach. The selection of the field for filtering is discussed for 2D filtered FDTD method and 2D filtered FD-FDTD Method with CFS-PML.

In order to find the optimized filtering wavenumber, Chapter 6 studies the numerical dispersion of the filtered FDTD method by assessing the numerical phase velocity error and introduces the major aspects that affect the stability and accuracy of the filtered FD-FDTD method with CFS-PML ABC. A practical example is demonstrated in Chapter 6 as well.

Chapter 7 concludes the dissertation and presents the possible future research works.

Appendix A implements the 3D spatial filtering approach. Spherical excitation is introduced for avoiding the high spatial frequency components which are generated from the single point excitation.
Chapter 2

Frequency-Dependent
Finite-Difference Time-Domain
Method

As a robust and accurate technique for solving the Maxwell’s equations in time domain, the finite-difference time-domain (FDTD) method is a widely used method to simulate the wave propagation of the various applications in the contemporary engineering. However, the dielectric parameters are specified as a constant in the conventional FDTD method, which ignores the dispersion property of the frequency-dependant (FD) materials. To overcome this drawback, the FD-FDTD method utilizes the material models like Debye model, Cole-Cole and other models to generate the dispersive materials for numerical computing [7]. This thesis uses the Debye model, which is simple in implementation and accurate in modeling the bio-tissues, for bio-electromagnetic applications. This chapter reviews the Maxwell’s equations and the FD-FDTD method with one-pole Debye model and complex-frequency-shifted perfectly matched layers (CFS-PML).

2.1 Maxwell’s equations

The Maxwell’s equations, which can be written in either integral form or differential form, interpret the interaction of the electricity and magnetism mathematically. The integral form presents the integral of the electromagnetic fields over a closed surface (or volume), which is sufficient for analytic calculations. Equivalent to the integral form in mathematics, the differential form describes amplitude of
the electromagnetic field at each point in both space and time. Thus, to display the wave propagation in the electromagnetic fields, the differential form of the Maxwell’s equations is a better choice than the integral form. In the regions without electromagnetic currents, the differential form of the time-varying Maxwell’s equations with absorbing materials are composed of the Faraday’s Law of

$$\frac{\partial B}{\partial t} = -\nabla \times E - J_m, \tag{2.1}$$

the Ampere’s Law of

$$\frac{\partial D}{\partial t} = \nabla \times H - J_e, \tag{2.2}$$

the Gauss’s Law for the electric field of

$$\nabla \cdot D = \rho \tag{2.3}$$

and the Gauss’s Law for the magnetic field of

$$\nabla \cdot B = 0 \tag{2.4}$$

where $E$ is the electric field vector, $H$ is the magnetic field vector, $D$ is the electric flux density vector, $B$ is the magnetic flux density vector, $J_m$ is the equivalent magnetic current density, $J_e$ is the electric current density and $\rho$ is the electric charge density. The Maxwell’s equations introduce two curl equations (2.1 and 2.2) and two divergence equations (2.3 and 2.4). The Faraday’s Law illustrates the physical phenomenon that a time-dependent magnetic field can create an electric field, and the Ampere’s Law expresses the reverse phenomenon of the Faraday’s Law. The Gauss’s Law for the electric field describes the relation between the electric charge density and the electric flux density. The Gauss’s Law for the magnetic field proves that magnetic monopoles do not exist. Therefore the total magnetic flux through a closed surface is zero.

The constitutive relations of the field-independent, direction-independent and frequency-independent materials are defined as

$$B = \mu H = \mu_0 \mu_r H, \tag{2.5}$$
\[ D = \epsilon E = \epsilon_0 \epsilon_r E, \]  
\[ (2.6) \]

\[ J_e = \sigma E \]  
\[ (2.7) \]

and

\[ J_m = \sigma^* H \]  
\[ (2.8) \]

where \( \epsilon \) is the electric permittivity, \( \epsilon_0 \) is the electric permittivity in free space, \( \epsilon_r \) is the relative electric permittivity, \( \mu \) is the magnetic permeability, \( \mu_0 \) is the magnetic permeability in free space, \( \mu_r \) is the relative magnetic permeability, \( \sigma \) is the electric conductivity and \( \sigma^* \) is the equivalent magnetic conductivity.

Substituting the constitutive relations from (2.5) to (2.8) into (2.1) and (2.2) yields

\[ \frac{\partial E}{\partial t} = \frac{1}{\epsilon} \nabla \times H - \frac{\sigma}{\epsilon} E \]  
\[ (2.9) \]

and

\[ \frac{\partial H}{\partial t} = -\frac{1}{\mu} \nabla \times E - \frac{\sigma^*}{\mu} H \]  
\[ (2.10) \]

which are the Maxwell’s curl equations for linear, isotropic and non-dispersive materials.

Applying (2.9) and (2.10) into the rectangular coordinate system, we obtain

\[ \frac{\partial E_x}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x \right), \]  
\[ (2.11) \]

\[ \frac{\partial E_y}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y \right), \]  
\[ (2.12) \]

\[ \frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right), \]  
\[ (2.13) \]
\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \sigma^* H_x \right), \quad (2.14)
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - \sigma^* H_y \right), \quad (2.15)
\]

and

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \sigma^* H_z \right). \quad (2.16)
\]

where \(E_x\) and \(H_x\) are electromagnetic field components in the \(x\)-direction, \(E_y\) and \(H_y\) are electromagnetic field components in the \(y\)-direction and \(E_z\) and \(H_z\) are electromagnetic field components in the \(z\)-direction.

### 2.2 Finite Difference Time Domain Method

#### 2.2.1 Finite Difference Approximation

The basic idea of the FDTD method is to discretize the Maxwell’s curl equations by using finite difference approximations. To estimate the field value at grid point \(x_0\), the finite difference approximation are derived from the forward Taylor expansion of

\[
f \left( x_0 + \frac{\Delta x}{2}, t \right) = f(x_0, t) + f'(x_0, t) \frac{\Delta x}{2} + \frac{f^{(2)}(x_0, t)}{2!} \left( \frac{\Delta x}{2} \right)^2 + \\
\quad \ldots + \frac{f^{(m)}(x_0, t)}{m!} \left( \frac{\Delta x}{2} \right)^m + \ldots (2.17)
\]

and the backward Taylor expansion of

\[
f \left( x_0 - \frac{\Delta x}{2}, t \right) = f(x_0, t) - f'(x_0, t) \frac{\Delta x}{2} + \frac{f^{(2)}(x_0, t)}{2!} \left( \frac{\Delta x}{2} \right)^2 - \\
\quad \ldots + (-1)^m \frac{f^{(m)}(x_0, t)}{m!} \left( \frac{\Delta x}{2} \right)^m + \ldots (2.18)
\]

where \(m\) is the order of polynomial, \(\Delta x\) is the discretized space size and \(f(x, t)\) is the one-dimensional wave solution that \(f(x, t) = e^{-j(kx-\omega t)}\) \((k\) is the wavenumber
and $\omega$ is the angular frequency). Subtracting (2.18) from (2.17) yields

$$f \left( x_0 + \frac{\Delta x}{2}, t \right) - f \left( x_0 - \frac{\Delta x}{2}, t \right) = f'(x_0, t) \Delta x + \frac{f^{(3)}(x_0, t)}{3} \left( \frac{\Delta x}{2} \right)^3 + \ldots$$

(2.19)

Dividing both sides of (2.19) by $\Delta x$ and then rearranging it, we derive the expression of central difference approximation as

$$\frac{\partial f(x_0, t)}{\partial x} = \frac{f \left( x_0 + \frac{\Delta x}{2}, t \right) - f \left( x_0 - \frac{\Delta x}{2}, t \right)}{\Delta x} - \frac{f^{(3)}(x_0, t)}{24} \Delta x^2 - \ldots$$

(2.20)

where $O(\Delta x^2)$ is the discretization error (or truncation error) which represents all the terms of order higher than two. The central difference approximation is explicit for updating the field value at next time step. Thus, by removing $O(\Delta x^2)$, Yee applied the central difference approximation with second order accurate to discretize the Maxwell’s curl equations.

Replacing the spatial interval $\Delta x^2$ in (2.17) by $\Delta x$, (2.17) can be manipulated as

$$\frac{\partial f(x_0, t)}{\partial x} = \frac{f \left( x_0 + \Delta x, t \right) - f \left( x_0, t \right)}{\Delta x} - O(\Delta x)$$

(2.21)

where $O(\Delta x)$ is the discretization error which represents the terms of order higher than one. (2.21) is the expression of forward difference approximation.

Similarly, from manipulation of (2.18), the backward difference approximation is obtained as

$$\frac{\partial f(x_0, t)}{\partial x} = \frac{f \left( x_0, t \right) - f \left( x_0 - \Delta x, t \right)}{\Delta x} - O(\Delta x).$$

(2.22)

The forward and backward difference approximations are first order accurate, if we remove the discretization error $O(\Delta x)$ of (2.21) and (2.22).

Equations (2.20), (2.21) and (2.22) are the difference equations for the first derivative of function $f(x)$ at grid $x_0$. To estimate the function $f(x)$ at $t_0$, we can use the semi-implicit approximation (central difference) of

$$f(x, t_0) = \frac{f \left( x, t_0 + \frac{\Delta t}{2} \right) + f \left( x, t_0 - \frac{\Delta t}{2} \right)}{2}.$$
2.2.2 Yee Algorithm

The finite difference scheme establishes the basis of the FDTD method to obtain the approximate solutions of the Maxwell’s curl equations at each point and time step. Reported by Yee [8], the FDTD method discretizes the electromagnetic fields by Yee cells and applies the leapfrog arrangement to update the fields information at each time step.

2.2.2.1 Yee Cell and Leapfrog Arrangement

As demonstrated in Figure 2.1, each electric field component of $E$ is surrounded by four magnetic field components of $H$, and each magnetic field component of $H$ is surrounded by four electric field components of $E$. According to their half
<table>
<thead>
<tr>
<th>Electromagnetic Component</th>
<th>Spatial Notation</th>
<th>Time Step</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>X-axis</td>
<td>Y-axis</td>
</tr>
<tr>
<td>$E_x$</td>
<td>$i + \frac{1}{2}$</td>
<td>$j$</td>
</tr>
<tr>
<td>$E_y$</td>
<td>$i$</td>
<td>$j + \frac{1}{2}$</td>
</tr>
<tr>
<td>$E_z$</td>
<td>$i$</td>
<td>$j$</td>
</tr>
<tr>
<td>$H_x$</td>
<td>$i$</td>
<td>$j + \frac{1}{2}$</td>
</tr>
<tr>
<td>$H_y$</td>
<td>$i + \frac{1}{2}$</td>
<td>$j$</td>
</tr>
<tr>
<td>$H_z$</td>
<td>$i + \frac{1}{2}$</td>
<td>$j + \frac{1}{2}$</td>
</tr>
</tbody>
</table>

Table 2.1: Notation of each electromagnetic field component in 3D.

space interval (noted in Table 2.1), the electric field components are placed in the middle of the cell edges and the magnetic field components are placed in the center of the cell faces. The Yee cell provides a solid geometry structure to obtain the solutions of the time-dependent Maxwell’s curl equations. This spatial arrangement of the electromagnetic components satisfies the physical properties of Faraday’s law and Ampere’s law [7].

Sampled alternatively in both time and space, the value of the electromagnetic field components are approximated by a set of difference equations. For example, the electric field component in time step $n + 1$ is updated by its information in the previous time step and the magnetic field component in time step $n + \frac{1}{2}$. This time marching procedure is called leapfrog arrangement.

### 2.2.2.2 Expression in Three-Dimension

Following the sampling information in Figure 2.1 and Table 2.1, the three-dimension FDTD method is derived by applying the finite difference equations into the scale equations from (2.11) to (2.16). For example [8][7], at time step $t = (n + \frac{1}{2})\Delta t$, the update equation for the electric field component $E_x$ at
\((i + \frac{1}{2}, j, k)\) is obtained by discretizing (2.11) to

\[
\frac{E^{n+\frac{1}{2}}(i+\frac{1}{2},j,k) - E^n(i+\frac{1}{2},j,k)}{\Delta t} = \frac{1}{\epsilon(i+\frac{1}{2},j,k)} \begin{pmatrix}
\frac{H_z^{n+\frac{1}{2}}(i+\frac{1}{2},\frac{j+\frac{1}{2}}{2},k) - H_z^{n+\frac{1}{2}}(i+\frac{1}{2},\frac{j-\frac{1}{2}}{2},k)}{\Delta y} \\
\frac{H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,\frac{k+\frac{1}{2}}{2}) - H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,\frac{k-\frac{1}{2}}{2})}{\Delta z} \\
\sigma(i + \frac{1}{2}, j, k) E_x^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k)
\end{pmatrix} .
\]

Based on the semi-implicit approximation (2.23), the difference form of the electric field component \(E_x^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k)\) at time step \(n + \frac{1}{2}\) is expressed as

\[
E_x^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k) = E_x^{n+1}(i + \frac{1}{2}, j, k) + E_x^n(i + \frac{1}{2}, j, k). \tag{2.25}
\]

Substituting (2.25) into equation (2.24) yields

\[
E_x^{n+1}(i+\frac{1}{2},j,k) - E^n(i+\frac{1}{2},j,k) = \frac{1}{\epsilon(i+\frac{1}{2},j,k)} \begin{pmatrix}
\frac{H_z^{n+\frac{1}{2}}(i+\frac{1}{2},\frac{j+\frac{1}{2}}{2},k) - H_z^n(i+\frac{1}{2},\frac{j-\frac{1}{2}}{2},k)}{\Delta y} \\
\frac{H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,\frac{k+\frac{1}{2}}{2}) - H_y^n(i+\frac{1}{2},j,\frac{k-\frac{1}{2}}{2})}{\Delta z} \\
\sigma(i + \frac{1}{2}, j, k) (E_x^{n+1}(i+\frac{1}{2},j,k) + E_x^n(i+\frac{1}{2},j,k))
\end{pmatrix} \tag{2.26}
\]

Rearranging (2.26) by collecting \(E_x^{n+1}(i + \frac{1}{2}, j, k)\) to the left side and the rest to the right side, we obtain

\[
E_x^{n+1}(i + \frac{1}{2}, j, k) = \begin{pmatrix}
1-\Delta t \frac{\sigma(i+\frac{1}{2},\frac{j}{2},k)}{2\epsilon(i+\frac{1}{2},\frac{j}{2},k)} \\
1+\Delta t \frac{\sigma(i+\frac{1}{2},\frac{j}{2},k)}{2\epsilon(i+\frac{1}{2},\frac{j}{2},k)} + E_x^n(i + \frac{1}{2}, j, k) \\
\frac{\Delta t}{\epsilon(i+\frac{1}{2},\frac{j}{2},k)} \\
\end{pmatrix} \begin{pmatrix}
H_z^{n+\frac{1}{2}}(i+\frac{1}{2},\frac{j+\frac{1}{2}}{2},k) - H_z^n(i+\frac{1}{2},\frac{j-\frac{1}{2}}{2},k) \\
H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,\frac{k+\frac{1}{2}}{2}) - H_y^n(i+\frac{1}{2},j,\frac{k-\frac{1}{2}}{2}) \\
\sigma(i + \frac{1}{2}, j, k)
\end{pmatrix} \tag{2.27}
\]

Equation (2.27) is the standard form of the Yee algorithm to update the electric component \(E_x\) at \(t = (n + 1) \Delta t\). Based on (2.12) and (2.13), the discretized
form of $E_y$ at $t = (n + 1) \Delta t$ is expressed as

$$
E_{y}^{n+1} \left( i, j + \frac{1}{2}, k \right) = \left( \begin{array}{c}
1 - \Delta t \frac{\sigma(i, j + \frac{1}{2}, k)}{2 \sigma(i, j + \frac{1}{2}, k)} \\
1 + \Delta t \frac{\sigma(i, j + \frac{1}{2}, k)}{2 \sigma(i, j + \frac{1}{2}, k)}
\end{array} \right) E_{y}^{n} \left( i, j + \frac{1}{2}, k \right) + \\
\left( \begin{array}{c}
\Delta t \\
\Delta z
\end{array} \right) \frac{H_{x}^{n+\frac{1}{2}}(i, j + \frac{1}{2}, k) - H_{x}^{n+\frac{1}{2}}(i, j + \frac{1}{2}, k - \frac{1}{2})}{\Delta z} \\
\frac{H_{x}^{n+\frac{1}{2}}(i, j + \frac{1}{2}, k - \frac{1}{2}) - H_{x}^{n+\frac{1}{2}}(i, j + \frac{1}{2}, k)}{\Delta x}
\end{array} \right)
$$

(2.28)

and $E_z$ at $t = (n + 1) \Delta t$ is expressed as

$$
E_{z}^{n+1} \left( i, j + \frac{1}{2}, k \right) = \left( \begin{array}{c}
1 - \Delta t \frac{\sigma(i, j, k + \frac{1}{2})}{2 \sigma(i, j, k + \frac{1}{2})} \\
1 + \Delta t \frac{\sigma(i, j, k + \frac{1}{2})}{2 \sigma(i, j, k + \frac{1}{2})}
\end{array} \right) E_{z}^{n} \left( i, j, k + \frac{1}{2} \right) + \\
\left( \begin{array}{c}
\Delta t \\
\Delta x
\end{array} \right) \frac{H_{y}^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k) - H_{y}^{n+\frac{1}{2}}(i - \frac{1}{2}, j, k + \frac{1}{2})}{\Delta x} \\
\frac{H_{y}^{n+\frac{1}{2}}(i + \frac{1}{2}, j + \frac{1}{2}, k) - H_{y}^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k)}{\Delta y}
\end{array} \right)
$$

(2.29)

Discretizing the equations (2.14), (2.15) and (2.16), the update equations for
the magnetic field components at \( t = (n + \frac{1}{2}) \Delta t \) are obtained as

\[
H_x^{n+\frac{1}{2}} (i, j + \frac{1}{2}, k + \frac{1}{2}) = \left( \begin{array}{c}
1 - \Delta t \frac{\sigma^*(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})} \\
1 + \Delta t \frac{\sigma^*(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}
\end{array} \right) \left( \begin{array}{c}
H_x^{n-\frac{1}{2}} (i, j + \frac{1}{2}, k + \frac{1}{2}) - \\
H_x^{n+\frac{1}{2}} (i, j + \frac{1}{2}, k + \frac{1}{2}) + \\
1 - \Delta t \frac{\Delta}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}
\end{array} \right).
\]

(2.30)

\[
H_y^{n+\frac{1}{2}} (i + \frac{1}{2}, j, k + \frac{1}{2}) = \left( \begin{array}{c}
1 - \Delta t \frac{\sigma^*(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})} \\
1 + \Delta t \frac{\sigma^*(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}
\end{array} \right) \left( \begin{array}{c}
H_y^{n-\frac{1}{2}} (i + \frac{1}{2}, j, k + \frac{1}{2}) - \\
H_y^{n+\frac{1}{2}} (i + \frac{1}{2}, j, k + \frac{1}{2}) + \\
1 - \Delta t \frac{\Delta}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2})}
\end{array} \right).
\]

(2.31)

and

\[
H_z^{n+\frac{1}{2}} (i + \frac{1}{2}, j + \frac{1}{2}, k) = \left( \begin{array}{c}
1 - \Delta t \frac{\sigma^*(i+\frac{1}{2}, j+\frac{1}{2}, k)}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k)} \\
1 + \Delta t \frac{\sigma^*(i+\frac{1}{2}, j+\frac{1}{2}, k)}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k)}
\end{array} \right) \left( \begin{array}{c}
H_z^{n-\frac{1}{2}} (i + \frac{1}{2}, j + \frac{1}{2}, k) - \\
H_z^{n+\frac{1}{2}} (i + \frac{1}{2}, j + \frac{1}{2}, k) + \\
1 - \Delta t \frac{\Delta}{2\mu(i+\frac{1}{2}, j+\frac{1}{2}, k)}
\end{array} \right).
\]

(2.32)
The finite-difference equations from (2.27) to (2.32) present the time marching algorithm of the electromagnetic field components in a Cartesian coordinate system. With the magnetic field components at \( t = (n - \frac{1}{2}) \Delta t \) and the electric field components at \( t = n\Delta t \), we can update the magnetic field to \( t = (n + \frac{1}{2})\Delta t \). Then with the electric field components at \( t = n\Delta t \) and the updated value of the magnetic field components at \( t = (n + \frac{1}{2})\Delta t \), the next time step of the electric field components is obtained by equations (2.27), (2.28) and (2.29).

### 2.2.2.3 Expression in Two-Dimension

To derive the equations for the two-dimensional FDTD method, we can remove the electric or magnetic vector components in one of the directions in the three-dimensional expression. Assuming the electric field components in \( z \)-direction are removed (\( E_z = 0 \)), the equations from (2.11) to (2.16) can be reduced to the transverse electric (TE) mode (only involves \( E_x \), \( E_y \) and \( H_z \)) of

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_z}{\partial y} - \sigma E_x \right),
\]

(2.33)

\[
\frac{\partial E_y}{\partial t} = \frac{1}{\epsilon} \left( -\frac{\partial H_z}{\partial x} - \sigma E_y \right)
\]

(2.34)

and

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \sigma^* H_z \right).
\]

(2.35)

When the \( z \)-direction components for the magnetic field (\( H_z = 0 \)) is removed, the transverse magnetic (TM) mode (only involves \( H_x \), \( H_y \) and \( E_z \)) is written as

\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left( -\frac{\partial E_z}{\partial y} - \sigma^* H_x \right),
\]

(2.36)

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} - \sigma^* H_y \right)
\]

(2.37)

and

\[
\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_x}{\partial x} - \frac{\partial H_y}{\partial y} - \sigma E_z \right).
\]

(2.38)
Figure 2.2: In 2D TE mode, the electric field components are located in the edge of the cell and the magnetic field components are located in the center of the the cell.

Figure 2.2 shows the two–dimensional Yee cell for the TE–mode and Table 2.2 is the notation of the electromagnetic field components of TE–mode. Therefore the discretized form of the TE mode are expressed as

\[
E_x^{n+1} \left( i + \frac{1}{2} , j \right) = \left( 1 - \Delta t \frac{\sigma(i+\frac{1}{2},j)}{2\epsilon(i+\frac{1}{2},j)} \right) E_x^n \left( i + \frac{1}{2} , j \right) \\
+ \left( \frac{\Delta t}{\epsilon(i+\frac{1}{2},j)} \right) \left( \frac{\Delta t}{2\epsilon(i+\frac{1}{2},j)} \right) \left( \frac{H_z^{n+\frac{1}{2}} (i + \frac{1}{2}, j + \frac{1}{2}) / \Delta y}{-H_z^{n+\frac{1}{2}} (i + \frac{1}{2}, j - \frac{1}{2}) / \Delta y} \right),
\]

(2.39)
Table 2.2: Notation of each electromagnetic field component in TE mode.

<table>
<thead>
<tr>
<th>Electromagnetic Component</th>
<th>Spatial Notation X-axis</th>
<th>Spatial Notation Y-axis</th>
<th>Time Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_x$</td>
<td>$i + \frac{1}{2}$</td>
<td>$j$</td>
<td>$n$</td>
</tr>
<tr>
<td>$E_y$</td>
<td>$i$</td>
<td>$j + \frac{1}{2}$</td>
<td>$n$</td>
</tr>
<tr>
<td>$H_z$</td>
<td>$i + \frac{1}{2}$</td>
<td>$j + \frac{1}{2}$</td>
<td>$n + \frac{1}{2}$</td>
</tr>
</tbody>
</table>

Table 2.3: Notation of each electromagnetic field component in TM mode.

<table>
<thead>
<tr>
<th>Electromagnetic Component</th>
<th>Spatial Notation X-axis</th>
<th>Spatial Notation Y-axis</th>
<th>Time Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_x$</td>
<td>$i$</td>
<td>$j + \frac{1}{2}$</td>
<td>$n + \frac{1}{2}$</td>
</tr>
<tr>
<td>$H_y$</td>
<td>$i + \frac{1}{2}$</td>
<td>$j$</td>
<td>$n + \frac{1}{2}$</td>
</tr>
<tr>
<td>$E_z$</td>
<td>$i$</td>
<td>$j$</td>
<td>$n$</td>
</tr>
</tbody>
</table>

\[ E_{y}^{n+1} \left( i, j + \frac{1}{2} \right) = \left( 1 - \Delta t \frac{\sigma(i,j+\frac{1}{2})}{2\epsilon(i,j+\frac{1}{2})} \right) \frac{1}{1 + \Delta t \frac{\sigma(i,j+\frac{1}{2})}{2\epsilon(i,j+\frac{1}{2})}} E_{y}^{n} \left( i, j + \frac{1}{2} \right) \]

\[ - \left( \frac{\Delta t}{\mu(i,j+\frac{1}{2})} \right) \left( \frac{1}{1 + \Delta t \frac{\sigma(i,j+\frac{1}{2})}{2\mu(i,j+\frac{1}{2})}} \right) \left( H_{z}^{n+\frac{1}{2}} \left( i + \frac{1}{2}, j + \frac{1}{2} \right) / \Delta x \right) - H_{z}^{n+\frac{1}{2}} \left( i - \frac{1}{2}, j + \frac{1}{2} \right) / \Delta x \right) \] (2.40)

and

\[ H_{z}^{n+\frac{1}{2}} \left( i + \frac{1}{2}, j + \frac{1}{2} \right) = \frac{1 - \Delta t \frac{\sigma^{*}(i+j+\frac{1}{2})}{2\mu(i+j+\frac{1}{2})}}{1 + \Delta t \frac{\sigma^{*}(i+j+\frac{1}{2})}{2\mu(i+j+\frac{1}{2})}} H_{z}^{n-\frac{1}{2}} \left( i + \frac{1}{2}, j + \frac{1}{2} \right) \]

\[ - \left( \frac{\Delta t}{\epsilon(i+j+\frac{1}{2})} \right) \left( \frac{1}{1 + \Delta t \frac{\sigma^{*}(i+j+\frac{1}{2})}{2\epsilon(i+j+\frac{1}{2})}} \right) \left( E_{y}^{n} \left( i + 1, j + \frac{1}{2} \right) / \Delta x \right) - E_{y}^{n} \left( i, j + \frac{1}{2} \right) / \Delta x - E_{x}^{n} \left( i + \frac{1}{2}, j + 1 \right) / \Delta y + E_{x}^{n} \left( i + \frac{1}{2}, j \right) / \Delta y \right) \]. (2.41)
Derived from (2.36), (2.37) and (2.38), with the notations in Table 2.3, the finite difference expression for TM mode are obtained as

\[
H_x^{n+\frac{1}{2}} (i, j + \frac{1}{2}) = \left( 1 - \frac{\Delta t \sigma^\ast (i, j + \frac{1}{2})}{2\mu (i, j + \frac{1}{2})} \right) \frac{H_x^n (i, j + \frac{1}{2})}{1 + \Delta t \sigma^\ast (i, j + \frac{1}{2})} - \left( \frac{\Delta t \mu (i, j + \frac{1}{2})}{1 + \Delta t \sigma^\ast (i, j + \frac{1}{2})} \right) \left( E_z^n (i, j + 1) / \Delta y \right) - E_z^n (i, j) / \Delta y
\]

(2.42)

\[
H_y^{n+\frac{1}{2}} (i + \frac{1}{2}, j) = \left( 1 - \frac{\Delta t \sigma^\ast (i + \frac{1}{2}, j)}{2\mu (i + \frac{1}{2}, j)} \right) \frac{H_y^n (i + \frac{1}{2}, j)}{1 + \Delta t \sigma^\ast (i + \frac{1}{2}, j)} + \frac{\Delta t \mu (i + \frac{1}{2}, j)}{1 + \Delta t \sigma^\ast (i + \frac{1}{2}, j)} \left( E_z^n (i + 1, j) / \Delta y \right) - E_z^n (i, j) / \Delta y
\]

(2.43)

and

\[
E_z^{n+1} (i, j) = \left( 1 - \frac{\Delta t \sigma (i, j)}{2\varepsilon (i, j)} \right) E_z^n (i, j)
\]

\[
+ \left( \frac{\Delta t \varepsilon (i, j)}{1 + \Delta t \sigma (i, j)} \right) \begin{pmatrix}
H_y^{n+\frac{1}{2}} (i + \frac{1}{2}, j) / \Delta x \\
- H_y^{n+\frac{1}{2}} (i - \frac{1}{2}, j) / \Delta x \\
- H_y^{n+\frac{1}{2}} (i, j + \frac{1}{2}) / \Delta y \\
+ H_y^{n+\frac{1}{2}} (i, j - \frac{1}{2}) / \Delta y
\end{pmatrix}
\]

(2.44)

### 2.2.2.4 Expression in one-Dimension

In the one-dimensional Cartesian coordinate system, let us assume the electromagnetic wave is only propagating along the z-direction. The Maxwell’s curl
equations from (2.11) to (2.16) are reduced to

\[
\frac{\partial E_x}{\partial t} = -\frac{1}{\epsilon} \left( \frac{\partial H_y}{\partial z} + \sigma E_x \right)
\] (2.45)

and

\[
\frac{\partial H_y}{\partial t} = -\frac{1}{\mu} \left( \frac{\partial E_x}{\partial z} + \sigma^* H_y \right).
\] (2.46)

This 1D mode only involves the field components \(E_x\) and \(H_y\). Following
the spatial notation in Table 2.4, the one-dimensional equations for the FDTD
method are derived as

\[
E_{x}^{n+1}(k) = \left( 1 - \Delta t \frac{\sigma(k)}{2\epsilon(k)} \right) E_{x}^{n}(k)
- \left( \frac{\Delta t}{1 + \Delta t \frac{\sigma(k)}{2\epsilon(k)}} \right) \left( H_{y}^{n+\frac{1}{2}} \left( k + \frac{1}{2} \right) / \Delta z - H_{y}^{n-\frac{1}{2}} \left( k - \frac{1}{2} \right) / \Delta z \right)
\] (2.47)

and

\[
H_{y}^{n+\frac{1}{2}} \left( k + \frac{1}{2} \right) = \left( 1 - \Delta t \frac{\sigma^*(k+\frac{1}{2})}{2\mu(k+\frac{1}{2})} \right) H_{y}^{n-\frac{1}{2}} \left( k + \frac{1}{2} \right)
- \left( \frac{\Delta t}{\mu(k+\frac{1}{2})} \right) \left( E_{x}^{n} \left( k + 1 \right) / \Delta z - E_{x}^{n} \left( k \right) / \Delta z \right)
\] (2.48)
2.3 Dispersive Materials

The electric permittivity of the dispersive material is complex and frequency-dependent. Thus, propagating in the dispersive medium, the electromagnetic waves with different frequencies have different phase velocities \[15\]. Regarding the media parameters as constants, the conventional FDTD method ignores the dielectric properties of the dispersive materials. Describing the material characteristics over a wide band of frequencies, many models like Debye model and Cole-Cole model, are developed for biological simulations. These two models can be adapted to different frequency ranges. The Debye model can accurately generate the material properties of the biological tissues for the frequencies which are higher than 1 GHz \[16\]. However, the Debye model is not sufficient to describe the media characteristics for the low frequencies, especially for frequencies below 10 MHz \[16\]. For such frequency range, the Cole-Cole model is a suggested alternative. This thesis uses the Debye model to simulate the dispersive materials for its accurate performance in the high frequency range. To simplify the implementation, the one-pole Debye relaxation model with auxiliary differential equations is adopted \[11\][17][18].

2.3.1 Debye Model

The constitutive relation for the electric flux density $D$ with dielectric materials is

$$D = \epsilon_0\epsilon_\infty E + P$$  \hspace{1cm} (2.49)

where $\epsilon_\infty$ is the relative permittivity at infinite frequency and $P$ is the electric polarization caused by dispersive materials which increase the total flux density \[19\][20]. For the linear material dispersion, the polarization $P$ is

$$P = \epsilon_0\chi_p E$$  \hspace{1cm} (2.50)
where $\chi_p$ is the electric susceptibility. $\chi_p$ is a function that can be expressed in either time domain or frequency domain. The dielectric dispersion is defined by the recursive convolution of $\chi_p(t)$ in time domain. Therefore, in the frequency domain, the frequency dependence of $\chi_p(\omega)$ must have a causal inverse Fourier transform from the time domain. Note that, the linear dispersion represents the linearity of the polarization $P$ to the electric field $E$, not the susceptibility $\chi_p$.

Substituting (2.7), (2.49) and (2.50) into Ampere’s Law (2.2) yields

$$\nabla \times H = (\epsilon_0 \epsilon_\infty + \epsilon_0 \chi_p) \frac{\partial E}{\partial t} + \sigma E$$

$$= (\epsilon_0 \epsilon_\infty + \epsilon_0 \chi_p) \frac{\partial E}{\partial t} + \sigma \frac{j\omega}{\epsilon_0} \frac{\partial E}{\partial t}$$

$$= \epsilon_0 \left( \epsilon_\infty + \chi_p + \frac{\sigma}{j\omega \epsilon_0} \right) \frac{\partial E}{\partial t}. \quad (2.51)$$

Equation (2.51) is adoptable for all kinds of the material models. The imaginary part of $(\epsilon_\infty + \chi_p + \frac{\sigma}{j\omega \epsilon_0})$ is the loss factor in the medium, and the real part determines how much energy can be stored into the medium from an external electric field.
For the one-pole Debye medium, the time domain form of the electric susceptibility is expressed as

\[ \chi_p(t) = \frac{\epsilon_s - \epsilon_\infty}{\tau_D} e^{-\frac{t}{\tau_D}} u(t) \] (2.52)

where \( \epsilon_s \) is the static relative permittivity, \( \tau_D \) is the characteristic relaxation time and \( u(t) \) is a function given by

\[ u(t) = \begin{cases} 
1, & t > 0 \\
0, & t \leq 0 
\end{cases} \] (2.53)

Figure 2.4 displays the susceptibility \( \chi_p(t) \) for the electric field with fat, which is generated by \( \epsilon_\infty = 3.9981, \epsilon_s = 5.5307 \) and \( \tau_D = 0.2363 \) ps. \( \chi_p(t) \) rises to its maximum value just after \( t = 0 \) and decreases to zero exponentially. The value of \( \chi_p(t) \) is zero before \( t = 0 \), thus the dispersive material at the FDTD grid is not excited before the wave arrives. To ensure the causality, the susceptibility \( \chi_p(\omega) \) in the frequency domain is derived as

\[ \chi_p(\omega) = \frac{\epsilon_s - \epsilon_\infty}{1 + j\omega\tau_D}. \] (2.54)

Substituting (2.54) into (2.51), Ampere’s Law for one-pole Debye medium can be rewritten as

\[ \nabla \times \mathbf{H} = \epsilon_0 \left( \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + j\omega\tau_D} + \frac{\sigma}{j\omega\epsilon_0} \right) \frac{\partial \mathbf{E}}{\partial t}. \] (2.55)

### 2.3.2 Formulations of the FD-FDTD method

The key point of the biomedical simulations is to generate the lossy biological medium for the microwave imaging, bio-electromagnetic hazard and other applications. Since the dispersive materials involve frequency-dependent dielectrics, the FD media can not be applied to the conventional FDTD method directly. There are two major techniques, the recursive convolution approach and the auxiliary differential equation (ADE) approach, that can implement the material models (like one-pole Debye model) to the time marching equation of the standard Yee algorithm. This thesis chooses the ADE scheme for its simplicity in implementation.
2.3.2.1 Recursive Convolution Scheme

In 1990 [20], Luebbers first derived the formulations of the FD-FDTD by using the recursive convolution scheme for Debye media. With the convolutional form of the polarization $P$, the flux density $D$ is written as [7][18][20]

$$ D = \epsilon_0 \epsilon_\infty E + P = \epsilon_0 \epsilon_\infty E + \int_{\tau=0}^{n\Delta t} E(t-\tau) \chi_p(\tau) d\tau. $$ (2.56)

Substituting (2.56) into Ampere’s Law (2.2), we can derive the update equations for the electric field $E$ with dispersive materials, which are presented in [20][21]. Although the recursive convolution approach can guarantee a second order accuracy for the FD-FDTD method, this approach requires a lot of floating-point operations and is only suitable for linear media.

2.3.2.2 Auxiliary Differential Equations

A simple implementation for the FD-FDTD method was reported in 1995 [22][23], which is called the ADE scheme. This ADE scheme requires less floating-point operations than the recursive convolution scheme. However, the memory usage of ADE is nearly twice as the recursive convolution method. Two years later [24], Okoniewski improved the ADE scheme for Debye model, which demands the same or less memory than the recursive convolution method.

According to Ampere’s Law for one-pole Debye model in (2.55), the ADE scheme assumes that the electric flux density $D$ is composed of the polarization $P$, the electric field component $E$ and the electric current density $J_e$, which is defined as

$$ D = \epsilon_0 \left( \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + j\omega \tau_D} + \frac{\sigma}{j\omega \epsilon_0} \right) E. $$ (2.57)

(2.57) can be rewritten as

$$ j^2 \omega^2 \tau_D D + j\omega D = j^2 \omega^2 \tau_D \epsilon_\infty \epsilon_0 E + j\omega (\sigma \tau_D + \epsilon_s \epsilon_0) E + \sigma E. $$ (2.58)

Then transforming (2.58) into the time domain, we obtain

$$ \frac{\partial^2 (\tau_D D)}{\partial t^2} + \frac{\partial D}{\partial t} = \frac{\partial^2 (\tau_D \epsilon_\infty \epsilon_0 E)}{\partial t^2} + \frac{\partial (\sigma \tau_D \epsilon_s \epsilon_0 E)}{\partial t} + \sigma E. $$ (2.59)
Thus the discretization form of (2.59) is expressed as

\[ E^{n+1} = S_1 E^n - S_2 E^{n-1} + S_3 D^{n+1} - S_4 D^n + S_5 D^{n-1} \]  

(2.60)

where

\[ S_1 = \frac{4\tau_D\epsilon_\infty\epsilon_0 + 2(\sigma\tau_D + \epsilon_s\epsilon_0)\Delta t - \sigma\Delta t^2}{2\tau_D\epsilon_\infty\epsilon_0 + 2(\sigma\tau_D + \epsilon_s\epsilon_0)\Delta t + \sigma\Delta t^2}, \]

\[ S_2 = \frac{2\tau_D\epsilon_\infty\epsilon_0}{2\tau_D\epsilon_\infty\epsilon_0 + 2(\sigma\tau_D + \epsilon_s\epsilon_0)\Delta t + \sigma\Delta t^2}, \]

\[ S_3 = \frac{2\tau_D + 2\Delta t}{2\tau_D\epsilon_\infty\epsilon_0 + 2(\sigma\tau_D + \epsilon_s\epsilon_0)\Delta t + \sigma\Delta t^2}, \]

\[ S_4 = \frac{4\tau_D + 2\Delta t}{2\tau_D\epsilon_\infty\epsilon_0 + 2(\sigma\tau_D + \epsilon_s\epsilon_0)\Delta t + \sigma\Delta t^2}, \]

and

\[ S_5 = \frac{2\tau_D}{2\tau_D\epsilon_\infty\epsilon_0 + 2(\sigma\tau_D + \epsilon_s\epsilon_0)\Delta t + \sigma\Delta t^2}. \]

Equation (2.60) is the ADE of the FD-FDTD method for updating \( E \). The equations for updating \( H \) are the same as (2.30), (2.31) and (2.32) for the FD-FDTD method. The time update equations for \( D \) are presented in [25]. To renew the electric field components at time step \( t = (n+1)\Delta t \), we need the information of the electric field and the electric flux density at \( t = n\Delta t \) and \( t = (n-1)\Delta t \), and the electric flux density at \( t = (n+1)\Delta t \). Therefore, to maintain the explicit computation, the time marching algorithm for the FD-FDTD method should follow the order of \( H^{n-\frac{1}{2}} \Rightarrow D^n \Rightarrow E^n \Rightarrow H^{n+\frac{1}{2}} \). The implementation of ADE requires two additional vector variables to store the field information of \( D \) and \( E \) in the time step which is two steps earlier than the next time step.
2.4 Perfectly Matched Layers

The perfect electrical conductor (PEC) boundary reflects all the outgoing waves for the conventional FDTD method, which bounds the electromagnetic components in a limited region. Simulating an infinite space in a truncated computational domain, the absorbing boundary condition (ABC) is developed to eliminate the wave reflections from the boundary \[20\] \[27\]. The Lindman boundary condition \[28\], Engquist-Majda boundary condition \[29\], Mur boundary condition \[30\], Bayliss boundary condition \[31\] and Liao boundary condition \[32\] are the most famous boundary conditions in 1970s and 1980s. All these ABCs adjust the value of the solutions at the edge of the grid by modifying the wave equations, and eliminate the reflections perfectly in the one dimensional scenario. In the two or three dimensional cases, since the reflections are generated at the boundary with different angles, these ABCs can only minimize the reflections but not absorb them completely \[33\]. Another remarkable drawback of these ABCs is that, the numerical calculation may become unstable with inhomogeneous medium \[7\].

As reported by Bérenger in 1994 \[34\], instead of modifying the wave equations, the perfectly matched layer (PML) ABC attenuates the traveling waves by inserting several PML layers, which are the layers of lossy materials (or PML materials). The impedance of the PML is perfectly matched between the PML and non-PML region, thus there are no spurious reflections at the interior-PML interface. Surrounded by the PML ABC, the computational domain can be terminated by the PEC boundary condition. The PML can absorb not only the outgoing wave from the interior-PML interface to the PEC boundary, but also the returning waves from the PEC boundary. To improve the absorbing ability of PML, we can simply increase the thickness of layers. The PML is efficient in absorbing the incident waves with different propagation angles and frequencies, and has a great capability for lossy, dispersive, inhomogeneous materials.

The implementations of PML are classified into two types, the split PML and un-split PML \[35\]. The split PML separates each field into two split-fields to solve the Maxwell’s equations in Cartesian coordinates \[34\] \[36\]. The un-split PML defines a special stretching coefficient to combine the split field components, which is a straightforward method to absorb the traveling waves. The un-split PML approaches, including the stretched-coordinate PML (SC-PML) \[37\], the uniaxial PML (UPML) \[38\] \[39\] \[40\] and the convolutional PML (CPML) \[12\] \[21\], keep the same propagation characteristics and reflection properties as the split
PML \[41\].

This thesis selects the CPML with complex frequency shifted (CFS) stretching coefficient (often called CFS-PML) to absorb the outgoing waves \[42\]. The CFS-PML is highly sufficient at absorbing the evanescent waves or very low frequency components \[43\][44\]. For the metric coefficients of the CFS-PML formulation are irrelevant to the material characteristics, the CFS-PML formulation is applicable for all kinds of material models \[7\].

### 2.4.1 Split PML

The Bérenger’s split PML is developed by separating the electromagnetic field components into two subcomponents. For example, \(E_x = E_{xy} + E_{xz}\), \(E_y = E_{yx} + E_{yz}\) and \(E_z = E_{zx} + E_{zy}\). Therefore (2.11) can be split to

\[
\epsilon \frac{\partial E_{xy}}{\partial t} + \sigma_y E_{xy} = \frac{\partial (H_{zx} + H_{zy})}{\partial y} \tag{2.61}
\]

and

\[
\epsilon \frac{\partial E_{xz}}{\partial t} + \sigma_z E_{xz} = - \frac{\partial (H_{yx} + H_{yz})}{\partial z} \tag{2.62}
\]

where \(\sigma_y\) and \(\sigma_z\) are the artificial PML conductivities. The remaining 10 split PML equations are derived from (2.12) to (2.16) \[35\]. Since the traveling wave is attenuated rapidly in the PML, it is usual to implement the PML by the exponential time difference rather than the central difference \[45\][46\]. The solution of the non-homogeneous differential equation (2.61) is composed of two parts \[47\][48\]. The first one is

\[
E_{xy_{gen}}(t) = \beta_1 e^{-\frac{\sigma_y}{\epsilon} t} \tag{2.63}
\]

where \(\beta_1\) is not equal to zero. (2.63) is the general solution of equation

\[
\frac{\partial E_{xy}}{\partial t} + \frac{\sigma_y}{\epsilon} E_{xy} = 0 \tag{2.64}
\]

which is the homogeneous differential equation that corresponds to (2.61). Based on (2.63), the electric field component \(E_{xy_{gen}}^{n+1}\) can be written as

\[
E_{xy_{gen}}^{n+1} = e^{-\frac{\sigma_y}{\epsilon} t} E_{xy_{gen}}^n. \tag{2.65}
\]
The second part of the solution of (2.61) is

\[ E_{xypar}(t) = \frac{1}{\sigma_y} \frac{\partial (H_{zx} + H_{zy})}{\partial y} + \beta_2 e^{-\sigma \epsilon t} \]  \hspace{1cm} (2.66)

which is a particular solution of (2.61) and \( \beta_2 \) is a coefficient that needs to be determined by the initial conditions. In the FDTD method, at \( t = 0 \), the electric field components are initialized as zero \( (E_{xypar}(t = 0) = 0) \). Thus (2.66) can be manipulated as

\[ 0 = \frac{1}{\sigma_y} \frac{\partial (H_{zx} + H_{zy})}{\partial y} + \beta_2 \]

\[ \therefore \beta_2 = -\frac{1}{\sigma_y} \frac{\partial (H_{zx} + H_{zy})}{\partial y}. \]  \hspace{1cm} (2.67)

Substituting the \( \beta_2 \) of (2.67) into (2.66), at the next step \( (t = \Delta t) \), we obtain

\[ E_{xypar}(\Delta t) = \frac{1}{\sigma_y} \left( 1 - e^{-\sigma \epsilon \Delta t} \right) \frac{\partial (H_{zx} + H_{zy})}{\partial y}. \]  \hspace{1cm} (2.68)

With the general solution of (2.65) and the particular solution of (2.68), the total increment of \( E_{xy} \) from \( t = n \Delta t \) to \( t = (n + 1) \Delta t \) is obtained as

\[ E_{xy}^{n+1} = e^{-\sigma \epsilon \Delta t} E_{xy}^n + \left( 1 - e^{-\sigma \epsilon \Delta t} \right) \frac{\sigma_y}{\sigma_y} \frac{\partial (H_{zx} + H_{zy})}{\partial y}. \]  \hspace{1cm} (2.69)

Substituting the notations in Table 2.1 into (2.69), the exponential discretization of (2.61) is expressed as

\[ E_{xy}^{n+1} \left( i + \frac{1}{2}, j, k \right) = \left( \begin{array}{c} \frac{-\sigma_y (i+\frac{1}{2}, j, k) \Delta t}{e^{-\sigma \epsilon (i+\frac{1}{2}, j, k) \Delta t}} \ E_{xy}^n \left( i + \frac{1}{2}, j, k \right) + \\
\frac{-\sigma_y (i+\frac{1}{2}, j, k) \Delta t}{\sigma_y (i+\frac{1}{2}, j, k) \Delta y} \ E_{xy}^n \left( i + \frac{1}{2}, j, k \right) \\
H_{zx}^{n+1/2} \left( i + \frac{1}{2}, j + \frac{1}{2}, k \right) + H_{zy}^{n+1/2} \left( i + \frac{1}{2}, j + \frac{1}{2}, k \right) - \\
H_{zx}^{n+1/2} \left( i + \frac{1}{2}, j - \frac{1}{2}, k \right) - H_{zy}^{n+1/2} \left( i + \frac{1}{2}, j - \frac{1}{2}, k \right) \end{array} \right). \]  \hspace{1cm} (2.70)
Equation (2.70) is the update equation for the $E_{xy}$ components in PML. The rest time marching equations can be derived by applying the exponential discretization to the split Maxwell’s equations, which are presented in [49].

2.4.2 Un-split PML

There are three major Un-split PMLs, the SC-PML, UPML and CFS-PML. Adopting the same absorbing medium as Bérenger’s PML, the SC-PML is a more effective implementation than the split PML. Based on the Maxwellian formulation, the UMPL applies an anisotropic medium to the FDTD method, which has the same absorbing performance as the split PML. Compared to the SC-PML and UPML, the CFS-PML has a better absorbing performance (the reflection is smaller), a stronger capability (efficient to absorb the evanescent waves or very low frequency components) and a simpler computational complexity (less memory requirement) [41] [50] [51]. Thus we implement the CFS-PML to absorb the outgoing waves of the FD-FDTD method. Since the CPML is developed from the SC-PML, let us start from the SC-PML.

2.4.2.1 Stretched-Coordinate PML

In [34], Bérenger pointed out that the PML can be realized with un-split electromagnetic fields, which is a straightforward implementation. Based on his idea, Chew and Weedon introduced a complex stretching coefficient to the split PML and derived a set of un-split equations. The implementation of Chew’s un-split PML is based on the stretched coordinate method [37].

Substituting the plane wave solutions of

$$E_{xy} = E_{0xy}e^{j\omega t - jk_x x - jk_y y - jk_z z}$$
and

$$E_{xz} = E_{0xz}e^{j\omega t - jk_x x - jk_y y - jk_z z}$$

(2.71)

into (2.61) and (2.62) yields

$$j\omega \epsilon (1 + \frac{\sigma_y}{j\omega \epsilon}) E_{xy} = \frac{\partial (H_{zx} + H_{zy})}{\partial y}$$
$$\therefore j\omega \epsilon \sigma_y(\omega) E_{xy} = \frac{\partial H_z}{\partial y}$$
$$\therefore j\omega \epsilon E_{xy} = \frac{1}{s_y(\omega)} \frac{\partial H_z}{\partial y}$$

(2.72)
and
\[ jw_\varepsilon (1 + \frac{\sigma_z}{jw_\varepsilon}) E_{xz} = -\frac{\partial (H_{yx} + H_{yz})}{\partial z} \]
\[ \therefore jw_\varepsilon s_z(\omega) E_{xz} = -\frac{\partial H_y}{\partial z} \]
\[ \therefore jw_\varepsilon E_{xz} = -\frac{1}{s_z(\omega)} \frac{\partial H_y}{\partial z} \]  \hspace{1cm} (2.73)

where \( k_x, k_y \) and \( k_z \) are the three-dimensional wavenumbers, and \( s_y(\omega) = 1 + \frac{\sigma_y}{jw_\varepsilon} \)
and \( s_z(\omega) = 1 + \frac{\sigma_z}{jw_\varepsilon} \) are the stretching coefficients of the split PML. The normalized
stretching coefficient is defined as
\[ s_I(\omega) = 1 + \frac{\sigma_I}{jw_\varepsilon} \quad \text{and} \quad s^*_I(\omega) = 1 + \frac{\sigma^*_I}{jw_\varepsilon} \]  \hspace{1cm} (2.74)

where \( I \) represents the directions. The combination of \( (2.72) \) and \( (2.73) \) yields
\[ jw_\varepsilon E_{xz} = \frac{1}{s_y(\omega)} \frac{\partial H_z}{\partial y} - \frac{1}{s_z(\omega)} \frac{\partial H_y}{\partial z} \]  \hspace{1cm} (2.75)

Transforming \( (2.75) \) to the time domain with a stretched coordinate \( [37] \), we obtain
\[ \epsilon \frac{\partial E_x}{\partial t} = s_y(t) \otimes \frac{\partial H_z}{\partial y} - s_z(t) \otimes \frac{\partial H_y}{\partial z} \]  \hspace{1cm} (2.76)

where \( \otimes \) signifies the convolution product and \( s_y(t) \) and \( s_z(t) \) are the inverse
Laplace transform of \( 1/s_y(\omega) \) and \( 1/s_z(\omega) \). \( (2.76) \) is an un-split Maxwell’s equation
for the \( E_x \) component. The equations for the remaining electromagnetic field
components are expressed as \([37]\)
\[ \epsilon \frac{\partial E_y}{\partial t} = s_z(t) \otimes \frac{\partial H_x}{\partial z} - s_x(t) \otimes \frac{\partial H_y}{\partial x} \]  \hspace{1cm} (2.77)
\[ \epsilon \frac{\partial E_z}{\partial t} = s_x(t) \otimes \frac{\partial H_y}{\partial x} - s_y(t) \otimes \frac{\partial H_x}{\partial y} \]  \hspace{1cm} (2.78)
\[ \epsilon \frac{\partial H_x}{\partial t} = s_y(t) \otimes \frac{\partial E_y}{\partial y} + s_x(t) \otimes \frac{\partial E_z}{\partial z} \]  \hspace{1cm} (2.79)
\[
\epsilon \frac{\partial H_y}{\partial t} = s^*_z(t) \otimes \frac{\partial E_x}{\partial z} + s^*_z(t) \otimes \frac{\partial E_z}{\partial x} \tag{2.80}
\]

and

\[
\epsilon \frac{\partial H_z}{\partial t} = s^*_x(t) \otimes \frac{\partial E_y}{\partial x} + s^*_y(t) \otimes \frac{\partial E_x}{\partial y}. \tag{2.81}
\]

Based on the equations from (2.76) to (2.81), Chew implemented the FD-FDTD method in [37]. Equations from (2.76) to (2.81) are the un-split Maxwell’s curl equations for both SC-PML and CFS-PML. The only difference between these two PML approaches is their stretching coefficient.

2.4.2.2 The CFS Stretching Coefficient

With the stretching coefficient in (2.74), the SC-PML is incapable of absorbing the very low frequency or evanescent waves [52][53]. To overcome this limitation, Kuzuoglu and Mittra inserted a degree of freedom \( \alpha \) into (2.74) to make the PML medium causal [42]. Thus the CFS stretching coefficients are defined as

\[
s_I(\omega) = \kappa_I + \frac{\sigma_I}{\alpha_I + j\omega\epsilon_0} \tag{2.82}
\]

and

\[
s^*_I(\omega) = \kappa_I + \frac{\sigma^*_I}{\alpha^*_I + j\omega\mu_0} \tag{2.83}
\]

where \( \kappa_I \) amplifies the attenuation of the incident wave, and \( \alpha_I \) is the key parameter that can enable or disable the absorbing ability of the CFS-PML [7]. Note that, \( \alpha_I \) is greater than zero, and \( \kappa_I \) is equal or greater than one. If \( \omega \gg \alpha_I/\epsilon_0 \), the CFS-PML absorbs the traveling waves as the standard PML. If \( \omega \ll \alpha_I/\epsilon_0 \), the imaginary part of the CFS stretching coefficient can be ignored and no wave attenuation happens in the CFS-PML.

2.4.2.3 The CFS-PML Formulation

The time domain equation of the convolutional CFS-PML is derived from the stretched coordinate equations from (2.76) to (2.81). Applying the inverse Laplace
transform to the CFS stretching coefficient in (2.82), we obtain

\[
\overline{\Sigma}_I(t) = \frac{\delta(t)}{\kappa_I} - \frac{\sigma_I}{\epsilon_0 \kappa_I^2} e^{-\frac{1}{\epsilon_0} (\kappa_I^2 + \alpha_I) t} u(t)
\]  

(2.84)

where \(\delta(t)\) is the Dirac function \([35]\). For non-dispersive media, substituting (2.84) into (2.76) yields

\[
\epsilon_0 \frac{\partial E_x}{\partial t} = \frac{1}{\kappa_y} \frac{1}{\kappa_z} \frac{1}{\kappa_z} \frac{\partial H_y}{\partial z} + \frac{\partial H_z}{\partial y} - \zeta_y(t) \otimes \frac{\partial H_z}{\partial y} - \zeta_z(t) \otimes \frac{\partial H_y}{\partial z}
\]

(2.85)

where

\[
\zeta_I(t) = -\frac{\sigma_I}{\epsilon_0 \kappa_I^2} e^{-\frac{1}{\epsilon_0} (\kappa_I^2 + \alpha_I) t} u(t).
\]

(2.86)

The discretization of (2.85) presents the explicit CFS-PML update equation for \(E_x\) of

\[
E_x^{n+1} = E_x^n + \frac{\Delta t}{\epsilon_0} \left[ \frac{\Delta H_z^{n+1/2}}{\Delta y} - \frac{\Delta H_y^{n+1/2}}{\Delta z} + \psi_{hz}^{n+1/2} - \psi_{hy}^{n+1/2} \right]
\]

(2.87)

where \(\psi_{hy}\) and \(\psi_{hz}\) are the discrete form of \(\zeta_i(t)\) convolved with the magnetic field components. They are realized by using the recursive convolution as

\[
\psi_{hz}^{n+1/2} = p_z \psi_{hz}^{n-1/2} + q_z \frac{\Delta H_y^{n+1/2}}{\Delta z}
\]

(2.88)

\[
\psi_{hy}^{n+1/2} = p_y \psi_{hy}^{n-1/2} + q_y \frac{\Delta H_z^{n+1/2}}{\Delta y}
\]

(2.89)

where

\[
p_I = e^{-\frac{\Delta t}{\epsilon_0} (\kappa_I^2 + \alpha_I) t}
\]

(2.90)

\[
q_I = \frac{\sigma_I}{\kappa_I (\kappa_I^2 + \kappa_I^2 \alpha_I)} (p_I - 1).
\]

(2.91)

Following the equations from (2.85) to (2.87), we can derive the update equations for \(E_y\) and \(E_z\) from (2.77) and (2.78). Based on the same procedure, the update equations for \(H_x\), \(H_y\) and \(H_z\) can be derived from (2.79), (2.80) and (2.81). In \([51]\), Gedney introduced a set of ADE equations to implement the CFS-PML, which is equivalent to the implementation in this section.
Chapter 3

Numerical Dispersion

The computational domain of the FDTD method is discretized by Yee cells in space and sampled by $\Delta t$ in time. As a nature of the numerical discretization, the numerical dispersion means that the phase velocity of the traveling wave in the FDTD grid is different from that in the physical world. The coarse spatial sampling causes delay and distortion, which can be accumulated and lead to incorrect simulation results, for the signals in the computational domain. Derived from the numerical dispersion relation, the Courant-Friedrich-Lewy (CFL) condition defines the upper bound of $\Delta t$ with respect to the spatial step size $\Delta x$, $\Delta y$ and $\Delta z$. For any $\Delta t$ greater than the CFL limit, the numerical waves are traveling faster than the speed of light in the FDTD domain. Therefore the solutions of the Maxwell’s curl equations are increased spuriously and the computation becomes unstable. Sections from 3.1 to 3.4 review the numerical dispersion, stability and phase velocity for the FDTD method. Section 3.5 presents the numerical dispersion relation for the CFS-PML and Section 3.6 derives the stability conditions of the CFS-PML.

3.1 Dispersion Relation for the Waves

The dispersion relation is a function that relates the frequency and wavenumber, which introduces the interrelationship for the electromagnetic waves propagating in the temporal and spatial domain.

The three-dimensional wave equation for homogeneous lossless medium is

$$\frac{\partial^2 f(x,y,z,t)}{\partial x^2} + \frac{\partial^2 f(x,y,z,t)}{\partial y^2} + \frac{\partial^2 f(x,y,z,t)}{\partial z^2} + \frac{\omega^2}{c^2} f(x,y,z,t) = 0$$

(3.1)
Figure 3.1: The three dimensional wavenumber \( \mathbf{k} \).

where \( c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \) is the speed of light and \( f_{(x,y,z,t)} \) is the wave solution of

\[
f_{(x,y,z,t)} = f_0 e^{-i(k_x x + k_y y + k_z z - \omega t)}.
\]  (3.2)

Substituting (3.2) into (3.1) yields

\[
(-k_x^2 - k_y^2 - k_z^2 + \frac{\omega^2}{c^2}) f_{(x,y,z,t)} = 0
\]

\[
k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{c^2}.
\]  (3.3)

Equation (3.3) is three dimensional dispersion relation for the electromagnetic waves. As shown in Figure 3.1, the three dimensional wavenumber is defined as

\( k_x = k \sin \theta \cos \varphi, \ k_y = k \sin \theta \sin \varphi \) and \( k_z = k \cos \theta \) (\( k \) is the amplitude, \( \theta \) and \( \varphi \) are the propagation angles), (3.3) can be simplified to

\[
k^2 = \frac{\omega^2}{c^2}.
\]  (3.4)

In (3.4), it is clear that the wavenumber is proportional to the frequency.
3.2 Numerical Dispersion

For an idealized space that has no electric and magnetic conductivities ($\sigma = 0$ and $\sigma^* = 0$), the time recursive equations from (2.27) to (2.32) are manipulated as

\[ E_{x, i+\frac{1}{2}, j, k}^{n+1} = E_x^n (i+\frac{1}{2}, j, k) \]

\[ + \frac{\Delta t}{\epsilon} \left( \frac{H_{z, i+\frac{1}{2}, j+\frac{1}{2}, k}^{n+\frac{1}{2}} - H_x^{n+\frac{1}{2}} (i+\frac{1}{2}, j+\frac{1}{2}, k)}{\Delta y} - \frac{H_{z, i+\frac{1}{2}, j, k}^{n+\frac{1}{2}} - H_x^{n+\frac{1}{2}} (i+\frac{1}{2}, j, k)}{\Delta z} \right) \] (3.5)

\[ E_{y, i, j+\frac{1}{2}, k}^{n+1} = E_y^n (i, j+\frac{1}{2}, k) \]

\[ + \frac{\Delta t}{\epsilon} \left( \frac{H_{z, i+\frac{1}{2}, j+\frac{1}{2}, k}^{n+\frac{1}{2}} - H_y^{n+\frac{1}{2}} (i+\frac{1}{2}, j+\frac{1}{2}, k)}{\Delta z} - \frac{H_{z, i, j+\frac{1}{2}, k}^{n+\frac{1}{2}} - H_y^{n+\frac{1}{2}} (i, j+\frac{1}{2}, k)}{\Delta x} \right) \] (3.6)

\[ E_{z, i, j, k+\frac{1}{2}}^{n+1} = E_z^n (i, j, k+\frac{1}{2}) \]

\[ + \frac{\Delta t}{\epsilon} \left( \frac{H_{y, i, j+\frac{1}{2}, k+\frac{1}{2}}^{n+\frac{1}{2}} - H_z^{n+\frac{1}{2}} (i, j+\frac{1}{2}, k+\frac{1}{2})}{\Delta x} - \frac{H_{y, i, j, k+\frac{1}{2}}^{n+\frac{1}{2}} - H_z^{n+\frac{1}{2}} (i, j, k+\frac{1}{2})}{\Delta y} \right) \] (3.7)

\[ H_{x, i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}}^{n+\frac{1}{2}} = H_x^{n+\frac{1}{2}} (i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}) \]

\[ - \frac{\Delta t}{\mu} \left( \frac{E_x^n (i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}) - E_x^n (i, j+\frac{1}{2}, k+\frac{1}{2})}{\Delta y} - \frac{E_y^n (i+\frac{1}{2}, j+\frac{1}{2}, k+1) - E_y^n (i, j+\frac{1}{2}, k+1)}{\Delta z} \right) \] (3.8)
\begin{equation}
H_{n+\frac{1}{2}}^{i+\frac{1}{2}, j, k+\frac{1}{2}} = H_{n-\frac{1}{2}}^{i+\frac{1}{2}, j, k+\frac{1}{2}} - \frac{\Delta t}{\mu} \left( \frac{E_x^n(i+\frac{1}{2}, j, k+1) - E_x^n(i+\frac{1}{2}, j, k)}{\Delta z} \right) - \left( \frac{E_x^n(i+1, j, k+\frac{1}{2}) - E_x^n(i, j, k+\frac{1}{2})}{\Delta x} \right) \tag{3.9}
\end{equation}

and

\begin{equation}
H_{z}^{n+\frac{1}{2}}(i+\frac{1}{2}, j + \frac{1}{2}, k) = H_{z}^{n-\frac{1}{2}}(i+\frac{1}{2}, j + \frac{1}{2}, k) - \frac{\Delta t}{\mu} \left( \frac{E_y^n(i+1, j+\frac{1}{2}, k) - E_y^n(i, j+\frac{1}{2}, k)}{\Delta y} \right) \tag{3.10}
\end{equation}

The discretized form of the wave solutions for the three dimensional electromagnetic wave are expressed as

\begin{equation}
E_{x}^n(i, j, k) = E_{x0} e^{-j(i\Delta x \tilde{k}_x + j\Delta y \tilde{k}_y + k\Delta z \tilde{k}_z - n\Delta t\omega)}, \tag{3.11}
\end{equation}

\begin{equation}
E_{y}^n(i, j, k) = E_{y0} e^{-j(i\Delta x \tilde{k}_x + j\Delta y \tilde{k}_y + k\Delta z \tilde{k}_z - n\Delta t\omega)}, \tag{3.12}
\end{equation}

\begin{equation}
E_{z}^n(i, j, k) = E_{z0} e^{-j(i\Delta x \tilde{k}_x + j\Delta y \tilde{k}_y + k\Delta z \tilde{k}_z - n\Delta t\omega)}, \tag{3.13}
\end{equation}

\begin{equation}
H_{x}^n(i, j, k) = H_{x0} e^{-j(i\Delta x \tilde{k}_x + j\Delta y \tilde{k}_y + k\Delta z \tilde{k}_z - n\Delta t\omega)}, \tag{3.14}
\end{equation}

\begin{equation}
H_{y}^n(i, j, k) = H_{y0} e^{-j(i\Delta x \tilde{k}_x + j\Delta y \tilde{k}_y + k\Delta z \tilde{k}_z - n\Delta t\omega)}, \tag{3.15}
\end{equation}

and

\begin{equation}
H_{z}^n(i, j, k) = H_{z0} e^{-j(i\Delta x \tilde{k}_x + j\Delta y \tilde{k}_y + k\Delta z \tilde{k}_z - n\Delta t\omega)} \tag{3.16}
\end{equation}

where \(\tilde{k}_x = \tilde{k} \sin \theta \cos \varphi\), \(\tilde{k}_y = \tilde{k} \sin \theta \sin \varphi\) and \(\tilde{k}_z = \tilde{k} \cos \theta\) are the components of the numerical wavevector in \(x\), \(y\) and \(z\) directions. Note that, \(\tilde{k}\) is the amplitude of numerical wavenumber.

Substituting the wave solutions (3.11), (3.15) and (3.16) into the discretized
Yee equation (3.5) yields
\[ e^{\Delta \omega - \frac{1}{2} \Delta x \tilde{k}_x} E^n_x (i, j, k) = e^{-\frac{1}{2} \Delta x \tilde{k}_x} E^n_x (i, j, k) \]
\[ + \frac{\Delta t}{\epsilon} \left( \frac{\Delta y}{\Delta z} \right) \left( e^{-\frac{1}{2} \Delta y \tilde{k}_y} - e^{\frac{1}{2} \Delta y \tilde{k}_y} \right) \left( e^{-\frac{1}{2} \Delta z \tilde{k}_z} - e^{\frac{1}{2} \Delta z \tilde{k}_z} \right) \].

(3.17)

(3.17) can be simplified to
\[ \left( e^{\frac{1}{2} \Delta t \omega} - e^{-\frac{1}{2} \Delta t \omega} \right) E^n_x (i, j, k) = \frac{\Delta t}{\epsilon} \left( \frac{\Delta y}{\Delta z} \right) \left( e^{-\frac{1}{2} \Delta y \tilde{k}_y} - e^{\frac{1}{2} \Delta y \tilde{k}_y} \right) \left( e^{-\frac{1}{2} \Delta z \tilde{k}_z} - e^{\frac{1}{2} \Delta z \tilde{k}_z} \right) \].

(3.18)

Applying Euler's formulae \( \sin x = \frac{e^{ix} - e^{-ix}}{2i} \) into (3.18), we obtain
\[ \sin \left( \frac{\Delta t \omega}{2} \right) E^n_x (i, j, k) = \frac{\Delta t}{\epsilon} \left( \frac{\Delta y}{\Delta z} \right) \left( \sin \left( \frac{\Delta y \tilde{k}_y}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \left( \sin \left( \frac{\Delta y \tilde{k}_y}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \].

(3.19)

Following the steps from equation (3.17) to (3.19), the discretized Yee equations from (3.6) to (3.10) can be rewritten as
\[ \sin \left( \frac{\Delta t \omega}{2} \right) E^n_y (i, j, k) = \frac{\Delta t}{\epsilon} \left( \sin \left( \frac{\Delta x \tilde{k}_x}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \left( \sin \left( \frac{\Delta x \tilde{k}_x}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \].

(3.20)

\[ \sin \left( \frac{\Delta t \omega}{2} \right) E^n_z (i, j, k) = \frac{\Delta t}{\epsilon} \left( \sin \left( \frac{\Delta y \tilde{k}_y}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \left( \sin \left( \frac{\Delta y \tilde{k}_y}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \].

(3.21)

\[ \sin \left( \frac{\Delta t \omega}{2} \right) H^n_x (i, j, k) = \frac{\Delta t}{\mu} \left( \sin \left( \frac{\Delta y \tilde{k}_y}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \left( \sin \left( \frac{\Delta y \tilde{k}_y}{2} \right) - \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) \right) \].

(3.22)
\[
\sin \left( \frac{\Delta t \omega}{2} \right) H_y^n(i, j, k) = \frac{\Delta t}{\mu} \left( \sin \left( \frac{\Delta z \tilde{k}_z}{2} \right) E_x^n(i, j, k) - \sin \left( \frac{\Delta x \tilde{k}_x}{2} \right) E_z^n(i, j, k) \right) 
\]
(3.23)

and

\[
\sin \left( \frac{\Delta t \omega}{2} \right) H_z^n(i, j, k) = \frac{\Delta t}{\mu} \left( \sin \left( \frac{\Delta x \tilde{k}_x}{2} \right) E_y^n(i, j, k) - \sin \left( \frac{\Delta y \tilde{k}_y}{2} \right) E_z^n(i, j, k) \right). 
\]
(3.24)

Based on the above six equations from (3.19) to (3.24), we obtain the three dimensional numerical dispersion relation of [7]

\[
\epsilon \mu \Delta t^2 \sin^2 \left( \frac{\Delta t \omega}{2} \right) = \sin^2 \left( \frac{\Delta x \tilde{k}_x}{2} \right) \Delta x^2 + \sin^2 \left( \frac{\Delta y \tilde{k}_y}{2} \right) \Delta y^2 + \sin^2 \left( \frac{\Delta z \tilde{k}_z}{2} \right) \Delta z^2.
\]
(3.25)

As discussed in Section 3.1, the dispersion relation (3.3) for the waves is linear. However, for the numerical dispersion (3.25), the relationship between the frequency and wavenumber is mainly governed by \(\Delta t, \Delta x, \Delta y\) and \(\Delta z\). According to l’Hospital’s rule, we can derive that \(\lim_{\Delta t \to 0} \frac{\sin(\Delta t \omega/2)}{\Delta t} = \frac{\omega}{2}\), \(\lim_{\Delta x \to 0} \frac{\sin(\Delta x \tilde{k}_x/2)}{\Delta x} = \frac{k_x}{2}\), \(\lim_{\Delta y \to 0} \frac{\sin(\Delta y \tilde{k}_y/2)}{\Delta y} = \frac{k_y}{2}\) and \(\lim_{\Delta z \to 0} \frac{\sin(\Delta z \tilde{k}_z/2)}{\Delta z} = \frac{k_z}{2}\). Thus if and only if \(\Delta t, \Delta x, \Delta y\) and \(\Delta z\) approach zero, the numerical dispersion equals the wave dispersion.

Based on the two dimensional FDTD equations from (2.42) to (2.44), the two dimensional dispersion equation is derived as

\[
\epsilon \mu \Delta t^2 \sin^2 \left( \frac{\Delta t \omega}{2} \right) = \sin^2 \left( \frac{\Delta x \tilde{k}_x}{2} \right) \Delta x^2 + \sin^2 \left( \frac{\Delta y \tilde{k}_y}{2} \right) \Delta y^2 
\]
(3.26)

where \(\tilde{k}_x = \tilde{k} \cos \varphi\) and \(\tilde{k}_y = \tilde{k} \sin \varphi\) are the 2D numerical wavenumbers. The 2D numerical wavenumbers are a special case of the 3D numerical wavenumbers with \(\cos \theta = 0\).

The one dimensional dispersion equation is derived from (2.47) and (2.48), where

\[
\frac{\sqrt{\epsilon \mu}}{\Delta t} \sin \left( \frac{\Delta t \omega}{2} \right) = \frac{\sin \left( \frac{\Delta x \tilde{k}_x}{2} \right)}{\Delta x} 
\]
(3.27)

where \(\tilde{k}_x = \tilde{k}\) is the 1D numerical wavenumber. The 1D numerical wavenumber

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is a special case of the 3D numerical wavenumbers with \( \cos \theta = 0 \) and \( \sin \varphi = 0 \).

### 3.3 Courant-Friedrichs-Lewy Condition

If the angular frequency is a complex value of \( \omega = \omega_{\text{real}} + j\omega_{\text{imag}} \), the wave solution (3.2) may either attenuate to zero \( (\omega_{\text{imag}} \text{ is positive}) \) or rise to infinity \( (\omega_{\text{imag}} \text{ is negative}) \) with respect to the time \( t \). Thus the amplitude of the wave depends on the value of \( \omega_{\text{imag}} \), which may cause instable wave behaviors. In order to ensure the stability, the angular frequency should be a real number and the term \( \sin \left( \frac{\Delta w}{2} \right) \) should be less than one. Then the numerical dispersion relation (3.25) can be written as

\[
\Delta t \leq \frac{1}{\sqrt{\varepsilon \mu}} \left( \frac{\sin \left( \frac{k_x \Delta x}{2} \right)}{\Delta x} \right)^2 + \left( \frac{\sin \left( \frac{k_y \Delta y}{2} \right)}{\Delta y} \right)^2 + \left( \frac{\sin \left( \frac{k_z \Delta z}{2} \right)}{\Delta z} \right)^2 \leq 1. \tag{3.28}
\]

(3.28) can be written as

\[
\Delta t \leq \frac{1}{\sqrt{\varepsilon \mu}} \sqrt{\left( \frac{\sin \left( \frac{k_x \Delta x}{2} \right)}{\Delta x} \right)^2 + \left( \frac{\sin \left( \frac{k_y \Delta y}{2} \right)}{\Delta y} \right)^2 + \left( \frac{\sin \left( \frac{k_z \Delta z}{2} \right)}{\Delta z} \right)^2}. \tag{3.29}
\]

Since the maximum value of the sinusoidal functions in (3.29) is one, thus the general form of (3.29) is \[55\] \[56\]

\[
\Delta t \leq \frac{\sqrt{\varepsilon \mu}}{\sqrt{3}}. \tag{3.30}
\]

If \( \Delta x = \Delta y = \Delta z \), (3.30) can be simplified to \( \Delta t \leq \frac{\Delta x \sqrt{\varepsilon \mu}}{\sqrt{3}} \). Inequality (3.30) is the Courant-Friedrichs-Lewy condition for the FDTD method, which defines the upper limit of \( \Delta t \) for stable computation. Based on (3.26), the CFL condition
for the two-dimensional case is

\[
\Delta t \leq \frac{\sqrt{\varepsilon \mu}}{\sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2}}.
\] (3.31)

If \( \Delta x = \Delta y \), (3.31) can be simplified to \( \Delta t \leq \frac{\Delta x \sqrt{\varepsilon \mu}}{2} \). Based on (3.27), the one-dimensional CFL condition is

\[
\Delta t \leq \frac{\sqrt{\varepsilon \mu}}{\sqrt{\Delta x}} = \Delta x \sqrt{\varepsilon \mu}.
\] (3.32)

In simulations, the wavenumber may become a complex value, if we set \( \Delta t \) greater than the upper limit of the CFL condition [7][57]. As a result, the phase velocity of the numerical wave may be faster than the speed of light and the amplitude of the wave in the FDTD grid increases exponentially [57].

### 3.4 Numerical Phase Velocity

Section 3.3 reviewed the CFL condition of the FDTD method to set the temporal size for stable computation. However, we can not set the Yee cell with any spatial size, even if \( \Delta t \) satisfies the CFL condition. The insufficient spatial sampling generates numerical dispersion, which causes incorrect numerical phase velocities. In the numerical calculation, the shortest wavelength of the excitation is \( \lambda_{\text{min}} = \frac{c}{f_{\text{highest}}} \), where \( f_{\text{highest}} \) is the highest frequency of the excitation. Thus, under the Nyquist sampling limit, the spatial size of each Yee cell should smaller than \( \Delta x = \lambda_{\text{min}}/2 \). However the Nyquist limit only guarantees the minimum accuracy for the FDTD computation and leads to large distortion for the numerical wave in different propagation angles. To improve the accuracy, more than two samples per minimum-wavelength is required. This section shows how to obtain the numerical phase velocity and measure the phase velocity error.
3.4.1 One Dimensional Phase Velocity

Based on the numerical dispersion relation in (3.27), the numerical wavenumber \( \tilde{k}_x \) can be derived as

\[
\tilde{k}_x = \frac{2}{\Delta x} \arcsin \left( \frac{\sqrt{\epsilon \mu} \Delta x}{\Delta t} \sin \left( \frac{\omega \Delta t}{2} \right) \right). \tag{3.33}
\]

Thus the 1D numerical phase velocity is defined as

\[
\tilde{c}_{1D} = \frac{\omega}{\tilde{k}_x} = \frac{\omega \Delta x}{2 \arcsin \left( \frac{\Delta x}{c \Delta t} \sin \left( \frac{\omega \Delta t}{2} \right) \right)}. \tag{3.34}
\]

We can analyze the numerical dispersion by comparing the numerical phase velocity with the physical phase velocity. Thus the 1D numerical phase velocity error is given by

\[
\mathcal{P}_{1D} = \left| \frac{c - \tilde{c}_{1D}}{c} \right| \tag{3.35}
\]

3.4.2 Two Dimensional Phase Velocity

In the two dimensional case, the electromagnetic wave involves a propagation angle \( \phi \). For the square Yee cell (\( \Delta x = \Delta y \)), the dispersion relation (3.26) in free space is rewritten as

\[
\left( \frac{\Delta x}{c \Delta t} \right)^2 \sin^2 \left( \frac{\Delta t \omega}{2} \right) = \sin^2 \left( \frac{\Delta x \tilde{k} \cos \phi}{2} \right) + \sin^2 \left( \frac{\Delta x \tilde{k} \sin \phi}{2} \right) \tag{3.36}
\]

If the numerical wave is propagating on the angles of \( \phi = 0, \phi = \pi/2, \phi = \pi \) and \( \phi = 3\pi/2 \), equation (3.36) can be reduced to

\[
\frac{\Delta x}{c \Delta t} \sin \left( \frac{\Delta t \omega}{2} \right) = \sin \left( \frac{\Delta x \tilde{k}}{2} \right). \tag{3.37}
\]

Then the numerical phase velocity for the wave propagating along the major...
grid axes is expressed as
\[
\tilde{c}_{2D_1} = \frac{\omega}{k} = \frac{\omega \Delta x}{2 \arcsin \left( \frac{\Delta x}{c \Delta t} \sin \left( \frac{\omega \Delta t}{2} \right) \right)}.
\] (3.38)

If the numerical wave is propagating on the angles of \( \varphi = \pi/4 \), \( \varphi = 3\pi/4 \), \( \varphi = 5\pi/4 \) and \( \varphi = 7\pi/4 \), equation (3.36) can be reduced to
\[
\frac{\Delta x}{c \Delta t} \sin \left( \frac{\Delta t \omega}{2} \right) = \sqrt{2} \sin \left( \frac{\Delta x k}{2 \sqrt{2}} \right).
\] (3.39)

Thus the numerical phase velocity for the wave propagating along the grid diagonals is expressed as
\[
\tilde{c}_{2D_2} = \frac{\omega}{k_x} = \frac{\omega \Delta x}{2 \sqrt{2} \arcsin \left( \frac{\Delta x}{c \Delta t \sqrt{2}} \sin \left( \frac{\omega \Delta t}{2} \right) \right)}.
\] (3.40)

Based on (3.38) and (3.40), the 2D numerical phase velocity error is given by
\[
\mathcal{P}_{2D} = \left| \frac{c - \min[\tilde{c}_{2D_1}, \tilde{c}_{2D_2}]}{c} \right|,
\] (3.41)
and the anisotropy error for the 2D FDTD method is
\[
\mathcal{P}_{2D_a} = \left| \frac{\tilde{c}_{2D_1} - \tilde{c}_{2D_2}}{\min[\tilde{c}_{2D_1}, \tilde{c}_{2D_2}]} \right|.
\] (3.42)

If \( \Delta t \) satisfies the CFL condition, the numerical phase velocity is always slower than the physical phase velocity. Thus \( \mathcal{P}_{2D} \) shows the loss of the wave propagation speed in numerical computations and \( \mathcal{P}_{2D_a} \) indicates the distortion of the traveling waves in the electromagnetic fields.

The Nyquist limit provides the maximum spatial size for each Yee cells. To improve the accuracy, we can minimize \( \Delta x \) to adequately sample the spatial field. Based on the numerical phase velocity error and anisotropy error, the sampling rate of at least ten cells per \( \lambda_{min} \) is often accepted [7].
3.5 Numerical Dispersion for PML

Equation (3.25) is the dispersion relation for the electromagnetic field with lossless materials, which is derived from the explicit central difference equations. In the lossy PML region, the amplitude of the signal is reduced rapidly. Therefore, in the PML, the central difference cannot sufficiently approximate the wave attenuation, especially in the first layers. Thus the PML introduces the exponential difference to discretize time steps of the electromagnetic fields.

3.5.1 One dimensional Dispersion

Derived from (2.9) and (2.10), the one dimensional Maxwell’s curl equations with PML conductivity are written as

\[ \frac{\epsilon}{c} \frac{\partial E_y}{\partial t} + \sigma_x E_y = -\frac{\partial H_z}{\partial x} \] (3.43)

and

\[ \mu \frac{\partial H_z}{\partial t} + \sigma^*_x H_z = -\frac{\partial E_y}{\partial x} \] (3.44)

where \( \sigma_x \) and \( \sigma^*_x \) is perfectly matched as \( \frac{\sigma_x}{\epsilon} = \frac{\sigma^*_x}{\mu} \). Applying the exponential difference for the partial differentials of time and central difference for the partial differentials of space to (3.43) and (3.44), the discretized PML equations with non-dispersive materials (\( \epsilon = \epsilon_0 \) and \( \mu = \mu_0 \)) are written as

\[ E^{n+1}_y (i) = a_x E^n_y (i) - b_x \frac{H_z^{n+\frac{1}{2}} (i + \frac{1}{2}) - H_z^{n+\frac{1}{2}} (i - \frac{1}{2})}{\Delta x} \] (3.45)

and

\[ H_z^{n+\frac{1}{2}} (i + \frac{1}{2}) = a^*_x H_z^{n-\frac{1}{2}} (i + \frac{1}{2}) - b^*_x \frac{E^n_y (i + 1) - E^n_y (i)}{\Delta x} \] (3.46)

where

\[ a_x = e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}, \quad a^*_x = e^{-\frac{\sigma^*_x \Delta t}{\mu_0}}. \] (3.47)
\[ b_I = \frac{1 - a_I}{\sigma_I} \quad \text{and} \quad b_I^* = \frac{1 - a_I^*}{\sigma_I^*}. \]  

(3.48)

The discretized wave solution for the \( x \)-directed electromagnetic waves are

\[ E^n_y (i) = E_{y0} e^{\omega n \Delta t - j k_x i \Delta x} \]  

(3.49)

and

\[ H^n_z (i) = H_{z0} e^{\omega n \Delta t - j k_x i \Delta x}. \]  

(3.50)

According to the PML’s matching condition \( (\sigma x \mu_0 = \sigma x^* \epsilon_0) \), we can derive \( a = a^* \) and \( b \epsilon_0 = b^* \mu_0 \) \[43\]. Then substitution of (3.49) and (3.50) into (3.45) and (3.46) yields

\[ e^{\omega \Delta t} E^n_y (i) = a_x E^n_y (i) - b_x \frac{e^{j j k_x \Delta x}}{\Delta x} \left( e^{-\frac{j j k_x \Delta x}{2}} - e^{-\frac{j j k_x \Delta x}{2}} \right) \]  

(3.51)

and

\[ e^{j j k_x \Delta x} e^{-\frac{j j k_x \Delta x}{2}} H^n_z (i) = a_x e^{-\frac{j j k_x \Delta x}{2}} e^{-\frac{j j k_x \Delta x}{2}} H^n_z (i) - b_x \frac{E^n_y (i)}{\Delta x} \left( e^{-j k_x \Delta x} - 1 \right). \]  

(3.52)

Reorganizing (3.51) by collecting \( E^n_y \) to the left hand side and the rest terms to the right hand side, then substituting this \( E^n_y \) into (3.52), the numerical dispersion relation for the one-dimensional PML is derived as

\[
\left( e^{j j k_x \Delta x} e^{-\frac{j j k_x \Delta x}{2}} - a_x e^{-\frac{j j k_x \Delta x}{2}} \right)^2 = b_x b_x^* \frac{j \hat{k}_x \Delta x}{\Delta x^2} \left( e^{-\frac{j j k_x \Delta x}{2}} - e^{-\frac{j j k_x \Delta x}{2}} \right)^2 = \left( 1 - a_x \right)^2 \frac{c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( e^{-\frac{j j k_x \Delta x}{2}} - e^{-\frac{j j k_x \Delta x}{2}} \right)^2 \]

(3.53)

If the matched conductivities \( \sigma x \) and \( \sigma x^* \) equal zero, then we can obtain that \( a_x = a_x^* = 1 \), \( b_x = \frac{\Delta t}{\Delta x} \) and \( b_x^* = \frac{\Delta t}{\mu_0} \) (L’Hôpital’s rule). Therefore, in the non-conductivities case, the dispersion relation (3.53) with the exponential discretization is equivalent to the one with central finite discretization in (3.27), although their time marching equations are different.
3.5.2 Two Dimensional Dispersion

The two dimensional dispersion can be derived from either the TE mode or TM mode. For example, the TM mode equations for the PML with non-dispersive materials are expressed as

\[ \varepsilon_0 \frac{\partial E_{zx}}{\partial t} + \sigma_x E_{zx} = \frac{\partial H_y}{\partial x}, \]  
(3.54)

\[ \varepsilon_0 \frac{\partial E_{zy}}{\partial t} + \sigma_y E_{zy} = -\frac{\partial H_x}{\partial y}, \]  
(3.55)

\[ \mu_0 \frac{\partial H_x}{\partial t} + \sigma^*_y H_x = -\frac{\partial (E_{zx} + E_{zy})}{\partial y}, \]  
(3.56)

and

\[ \mu_0 \frac{\partial H_y}{\partial t} + \sigma^*_x H_y = \frac{\partial (E_{zx} + E_{zy})}{\partial x}. \]  
(3.57)

Applying the exponential and central difference approximation, the discretization of (3.54), (3.55), (3.56) and (3.57) yields

\[ E_{zx}^{n+1}(i,j) = a_x E_{zx}^n(i,j) + b_x \frac{H_y^{n+\frac{1}{2}} (i + \frac{1}{2}) - H_y^{n-\frac{1}{2}} (i - \frac{1}{2})}{\Delta x}, \]  
(3.58)

\[ E_{zy}^{n+1}(i,j) = a_y E_{zy}^n(i,j) - b_y \frac{H_x^{n+\frac{1}{2}} (i + \frac{1}{2}) - H_x^{n-\frac{1}{2}} (i - \frac{1}{2})}{\Delta y}, \]  
(3.59)

\[ -\frac{b_y}{\Delta y} [E_{zx}^n(i, j + 1) + E_{zy}^n(i, j + 1) - E_{zx}^n(i, j) - E_{zy}^n(i, j)] \]  
(3.60)

and

\[ H_x^{n+\frac{1}{2}}(i, j + \frac{1}{2}) = a_y H_x^{n-\frac{1}{2}}(i, j + \frac{1}{2}) \]  

\[ H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j) = a_x H_y^{n-\frac{1}{2}}(i + \frac{1}{2}, j) \]  

\[ + \frac{b_x}{\Delta x} [E_{zx}^n(i + 1, j) + E_{zy}^n(i + 1, j) - E_{zx}^n(i, j) - E_{zy}^n(i, j)]. \]  
(3.61)
Applying the discrete wave solutions of

\[ E^n_{zz}(i,j) = E_{zz0} e^{\omega_n \Delta t - \tilde{k}_x i \Delta x - \tilde{k}_y j \Delta y}, \]  
(3.62)

\[ E^n_{zy}(i,j) = E_{zy0} e^{\omega_n \Delta t - \tilde{k}_x i \Delta x - \tilde{k}_y j \Delta y}, \]  
(3.63)

\[ H^n_x(i,j) = H_{x0} e^{\omega_n \Delta t - \tilde{k}_x i \Delta x - \tilde{k}_y j \Delta y} \]  
(3.64)

and

\[ H^n_y(i,j) = H_{y0} e^{\omega_n \Delta t - \tilde{k}_x i \Delta x - \tilde{k}_y j \Delta y} \]  
(3.65)

into (3.58), (3.59), (3.60) and (3.61), we obtain

\[ e^{\omega \Delta t} E^n_{zz}(i,j) = a_x E^n_{zz}(i,j) + b_x \frac{e^{\frac{1}{2} \omega \Delta t} H^n_y(i)}{\Delta x} \left( e^{-\frac{1}{2} \tilde{k}_y \Delta y} - e^{\frac{1}{2} \tilde{k}_y \Delta y} \right), \]  
(3.66)

\[ e^{\omega \Delta t} E^n_{zy}(i,j) = a_y E^n_{zy}(i,j) - b_y \frac{e^{\frac{1}{2} \omega \Delta t} H^n_x(i)}{\Delta y} \left( e^{-\frac{1}{2} \tilde{k}_x \Delta x} - e^{\frac{1}{2} \tilde{k}_x \Delta x} \right), \]  
(3.67)

\[ e^{\frac{1}{2} \omega \Delta t} e^{-\frac{1}{2} \tilde{k}_y \Delta y} H^n_x(i,j) = e^{-\frac{1}{2} \omega \Delta t} e^{-\frac{1}{2} \tilde{k}_y \Delta y} a_y^* H^n_x(i,j) \]  
\[ - b_y \frac{e^{\frac{1}{2} \omega \Delta t} E^n_{zz}(i,j) + E^n_{zy}(i,j)}{\Delta y} \left( e^{-\tilde{k}_y \Delta y} - 1 \right) \]  
(3.68)

and

\[ e^{\frac{1}{2} \omega \Delta t} e^{-\frac{1}{2} \tilde{k}_x \Delta x} H^n_y(i,j) = e^{-\frac{1}{2} \omega \Delta t} e^{-\frac{1}{2} \tilde{k}_x \Delta x} a_x^* H^n_y(i,j) \]  
\[ + b_x \frac{E^n_{zz}(i,j) + E^n_{zy}(i,j)}{\Delta x} \left( e^{-\tilde{k}_x \Delta x} - 1 \right). \]  
(3.69)

Then substitution of (3.68) and (3.69) into (3.67) and (3.66) yields

\[ \left( e^{\frac{1}{2} \omega \Delta t} - a_x e^{-\frac{1}{2} \omega \Delta t} \right)^2 E^n_{zz}(i,j) \]  
\[ = \frac{(1 - a_x)^2 \sigma_x^2 \Delta x^2}{(\nu^2 + \omega^2) \Delta x^2} \left( e^{-\frac{1}{2} \tilde{k}_x \Delta x} - e^{\frac{1}{2} \tilde{k}_x \Delta x} \right)^2 \left( E^n_{zz}(i,j) + E^n_{zy}(i,j) \right) \]  
(3.70)
and

\[
\left( e^{j\frac{1}{2}\Delta t} - ay e^{-j\frac{1}{2}\Delta t} \right)^2 E^n_{zy}(i,j) = \frac{(1 - ay)^2 c^2 \epsilon_0^2}{\sigma_y^2 \Delta y^2} \left( e^{-j\frac{1}{2}ky \Delta y} - e^{j\frac{1}{2}ky \Delta y} \right)^2 \left( E^n_{zx}(i,j) + E^n_{zy}(i,j) \right). \tag{3.71}
\]

Reorganizing (3.70) by collecting \( E^n_{zx} \) to the left side and the rest terms to the right side, then substituting this \( E^n_{zx} \) into (3.71), the numerical dispersion relation for two-dimensional PML is derived as

\[
\frac{(1 - ax)^2 c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( e^{-j\frac{1}{2}kx \Delta x} - e^{j\frac{1}{2}kx \Delta x} \right)^2 \left( e^{j\frac{1}{2}\omega \Delta t} - ax e^{-j\frac{1}{2}\omega \Delta t} \right)^2 \tag{3.72}
\]

\[
+ \frac{(1 - ay)^2 c^2 \epsilon_0^2}{\sigma_y^2 \Delta y^2} \left( e^{-j\frac{1}{2}ky \Delta y} - e^{j\frac{1}{2}ky \Delta y} \right)^2 \left( e^{j\frac{1}{2}\omega \Delta t} - ax e^{-j\frac{1}{2}\omega \Delta t} \right)^2 = \left( e^{j\frac{1}{2}\omega \Delta t} - ax e^{-j\frac{1}{2}\omega \Delta t} \right)^2 \left( e^{j\frac{1}{2}\omega \Delta t} - ay e^{-j\frac{1}{2}\omega \Delta t} \right)^2.
\]

### 3.6 Further Investigation for the Dispersion of CFS-PML

It is a challenge to derive the stability condition for the PML, since the complex stretching coefficient of the PML generates a complex wavenumber. Thus it is usual to evaluate the stability of PML by numerical experiments. Based on the dispersion relations in Section 3.5, this section presents some conditions to determine the temporal size of the 1D and 2D CFS-PML.

#### 3.6.1 Investigation for One Dimensional Dispersion

The CFS-PML has an additional matched condition, which is \( \alpha_x \mu_0 = \alpha_x^* \epsilon_0 \). If \( \kappa_x = \kappa_x^* \), the one dimensional wavenumber in the CFS-PML is expressed as

\[
\tilde{k}_x = \frac{\omega}{c} \sqrt{s_x s_x^*} = \frac{\omega}{c} \left( \kappa_x + \frac{\sigma_x}{\alpha_x + j\omega \epsilon_0} \right). \tag{3.73}
\]
Substituting (3.73) into (3.53), we obtain
\[
\left( \frac{j \omega \Delta t}{2} - a_x e^{-\frac{j \omega \Delta t}{2}} \right)^2 = \left( \frac{1 - a_x}{\sigma_x^2 \Delta x^2} \right)^2 \left( e^{\frac{\Delta x \omega}{2c}} \frac{A}{2c} e^{\frac{\Delta x \omega}{2c} B} - e^{-\frac{\Delta x \omega}{2c}} e^{-\frac{\Delta x \omega}{2c} B} \right)^2
\]  
(3.74)

where
\[
A = \kappa_x + \frac{\sigma_x \alpha_x}{\alpha_x^2 + \omega^2 \epsilon_0^2} \quad \text{and} \quad B = \frac{\omega \sigma_x \epsilon_0}{\alpha_x^2 + \omega^2 \epsilon_0^2}.
\]  
(3.75)

Application of Euler’s formulae \((e^{jx} = \cos x + j \sin x)\) to (3.74) yields
\[
\left( (1 - a_x) \cos \left( \frac{\omega \Delta t}{2} \right) + j (1 + a_x) \sin \left( \frac{\omega \Delta t}{2} \right) \right)^2 = \left( \frac{(1 - a_x)^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi - \Psi^{-1}) \cos \left( \frac{\Delta x \omega}{2c} A \right) + j(\Psi + \Psi^{-1}) \sin \left( \frac{\Delta x \omega}{2c} A \right) \right) \right)^2
\]  
(3.76)

where
\[
\Psi = e^{\frac{\Delta x \omega}{2c}} B.
\]  
(3.77)

Equation (3.76) can be separated into a real part equation of
\[
(1 + a_x^2)(2 \cos^2 \left( \frac{\omega \Delta t}{2} \right) - 1) - 2a_x =
\]
\[
\left( \frac{(1 - a_x)^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi^2 + \Psi^{-2})(2 \cos^2 \left( \frac{\Delta x \omega}{2c} A \right) - 1) - 2 \right) \right)
\]  
(3.78)

and an imaginary part equation of
\[
(1 - a_x^2) \sin(\omega \Delta t) = \left( \frac{(1 - a_x)^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} (\Psi^2 - \Psi^{-2}) \sin \left( \frac{\Delta x \omega}{c} A \right) \right).
\]  
(3.79)

### 3.6.1.1 Manipulation of (3.78)

Since \(0 \leq \cos^2 \left( \frac{\omega \Delta t}{2} \right) \leq 1\), the real part equation (3.78) can be written as
\[
-(1 + a_x)^2 \leq \left( \frac{(1 - a_x)^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi^2 + \Psi^{-2})(2 \cos^2 \left( \frac{\Delta x \omega}{2c} A \right) - 1) - 2 \right) \right) \leq (1 - a_x)^2.
\]  
(3.80)
In the absence of PML conductivity ($\sigma_x = 0$), Equation (3.80) is always satisfied since $a_x$ equals to one. However the term $(1 - a_x)$ does not equal zero in the CFS-PML, and Equation (3.80) can be divided into two conditions. The first one is

$$X_A \triangleq \frac{c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi^2 + \Psi^{-2}) \cos \left( \frac{\Delta x \omega_c}{c} A \right) - 2 \right) \leq 1 \quad (3.81)$$

and the second one is

$$0 \leq \left( \frac{1 - a_x}{1 + a_x} \right)^2 \frac{c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi^2 + \Psi^{-2}) \cos \left( \frac{\Delta x \omega_c}{c} A \right) - 2 \right) + 1 \triangleq Y_A. \quad (3.82)$$

Figure 3.2: $X_A$ varying $\frac{\Delta x \omega_c}{c}$ from zero to $\pi$ for the cases of $\Delta x = 2$ mm, $\Delta x = 1$ mm and $\Delta x = 0.5$ mm.

Let us define the left hand side of (3.81) as $X_A$, the right hand side of (3.82) as $Y_A$ and the maximum temporal size for stable computation in the 1D FDTD method as $\Delta t_{cfl1d}$.

Since $\sigma_x$ should be a positive number and $\kappa_x$ should be equal to or greater than one [35, 51, 59], let us set $\sigma_x = 0.001$, $\kappa_x = 1$ and $a_x = 0.0016$ to calculate the value of $X_A$. Figure 3.2 displays the variations of $X_A$ with $\frac{\Delta x \omega_c}{c}$ for the cases of $\Delta x = 2$ mm, $\Delta x = 1$ mm and $\Delta x = 0.5$ mm. According to the Nyquist
sampling theorem, the greatest $\frac{\Delta x \omega}{c}$ in numerical simulation is $\pi$. Thus we plot Figure 3.2 in the range of $0 \leq \frac{\Delta x \omega}{c} \leq \pi$. In Figure 3.2 with the parameters of $\sigma_x = 0.001, \kappa_x = 1$ and $\alpha_x = 0.0016$, $\mathcal{X}_A$ is smaller than one, which satisfies the condition in (3.81). Therefore this set of parameters is used to generate the stretching coefficient of CFS-PML in later calculations and simulations.

The maximum value of $\mathcal{X}_A$ is obtained when $\cos(\frac{\Delta x \omega}{c} \mathcal{A}) = 1$. Therefore (3.81) can be further manipulated to

$$\frac{c^2 \epsilon_0}{\sigma_x^2 \Delta x^2} (\Psi^2 + \Psi^{-2} - 2) \leq 1. \quad (3.83)$$

Since $a_x$ is a function of $\Delta t$, we plot $\mathcal{Y}_A$ with several values of $\Delta t$ for the case of $\Delta x = 1$ mm in Figure 3.3. According to the results in Figure 3.3, $\mathcal{Y}_A$ is greater than zero if $\Delta t$ is equal to or smaller than $\Delta t_{cfl1d}$. In further calculations, the results of using $\Delta x = 2$ mm and $\Delta x = 0.5$ mm are identical to the results in Figure 3.3, which proves that the change of $\Delta x$ does not affect the value of $\mathcal{Y}_A$. The lower bound of $\mathcal{Y}_A$ takes place at $\frac{\Delta x \omega}{c} \mathcal{A} = \pi$. Then condition (3.82) can be
further manipulated as

\[
\left( \frac{1 - a_x}{1 + a_x} \right)^2 \frac{c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right)^2 \leq 1.
\]  

(3.84)

Substituting (3.47) into (3.84) yields

\[
\left( \frac{1 - e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}}{1 + e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}} \right)^2 \frac{c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right)^2 \leq 1
\]

\[
\therefore \frac{1 - e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}}{1 + e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}} \leq \frac{c\epsilon_0}{\sigma_x \Delta x} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right)
\]

\[
\therefore \frac{2 \frac{c\epsilon_0}{\sigma_x \Delta x} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right)}{1 + e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}} \leq 1 + e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}
\]

\[
\therefore e^{-\frac{\sigma_x \Delta t}{\epsilon_0}} \leq \frac{\frac{c\epsilon_0}{\sigma_x \Delta x} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right) + 1}{\frac{c\epsilon_0}{\sigma_x \Delta x} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right) - 1}
\]

\[
\therefore \Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left( \frac{\frac{c\epsilon_0}{\sigma_x \Delta x} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right) + 1}{\frac{c\epsilon_0}{\sigma_x \Delta x} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right) - 1} \right).
\]

(3.85)

Since \( \Delta t \) is a real number, the term \( \frac{c\epsilon_0}{\sigma_x \Delta x} \left( e^{\frac{x_B}{\Delta x}} + e^{-\frac{x_B}{\Delta x}} \right) \) in (3.85) should be greater than one.

### 3.6.1.2 Manipulation of (3.79)

In numerical calculation, \( \sin(\omega \Delta t) \) is a positive number from zero to one for \( 0 \leq \omega \Delta t \leq \pi \). Thus (3.79) can be written as

\[
0 \leq \frac{(1 - a_x)^2}{\sigma_x^2 \Delta x^2} \frac{c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} (\Psi^2 - \Psi^{-2}) \sin\left( \frac{\Delta x \omega c}{\epsilon} \right) \leq (1 - a_x^2).
\]

(3.86)
\[
\Delta t_{pml} = \frac{c^2 \epsilon_0^2}{\sigma^2 \Delta x^2} (\Psi^2 - \Psi^{-2}) \sin\left(\frac{\Delta x \omega}{c} A\right) + 1
\]

\[
\Delta t_{cfl_{1d}} \leq \Delta t_{pml}.
\]

Note that, \(\frac{c^2 \epsilon_0^2}{\sigma^2 \Delta x^2} (\Psi^2 - \Psi^{-2}) \sin\left(\frac{\Delta x \omega}{c} A\right)\) should be greater than one in (3.88).

Equation (3.88) defines the upper limit of \(\Delta t\) for stable computation with CFS-PML ABC. Let us define the right hand side of (3.88) as \(\Delta t_{pml}\). In order to use any \(\Delta t\) under the CFL condition for CFS-PML, \(\Delta t_{pml}\) should be equal to or greater than \(\Delta t_{cfl_{1d}}\) for any \(\frac{\Delta x \omega}{c}\) from zero to \(\pi\). Otherwise the computation may
suffer from the late-time instability. \( \Delta t_{pml} \) can be further manipulated as

\[
\Delta t_{pml} = \frac{\epsilon_0}{\sigma_x} \ln \left( 1 + \frac{2}{c^2 \epsilon_0 \sigma_x (\Psi^2 - \Psi^{-2}) \sin(\frac{\Delta x}{c} A)} \right)
\] (3.89)

which indicates that, \( \Delta t_{pml} \) decreases with increasing \((\Psi^2 - \Psi^{-2}) \sin(\frac{\Delta x}{c} A)\). However, in the range of \(0 \leq \frac{\Delta x c}{\omega} \leq \pi\), the maximum value of \((\Psi^2 - \Psi^{-2}) \sin(\frac{\Delta x}{c} A)\) takes place at \(\frac{\Delta x c}{\omega} = \pi\), while \(\sin(\frac{\Delta x}{c} A)\) takes its maximum value at \(\frac{\Delta x}{c} A = \frac{\pi}{2}\). Thus the minimum value of \(\Delta t_{pml}\) is in the range of \(\frac{\pi}{2} A < \frac{\Delta x c}{\omega} < \pi\). With the parameters of CFS-PML which are used to produce Figure 3.2, Figure 3.4 compares \(\Delta t_{pml}\) with \(\Delta t_{cfl,1d}\), and shows that \(\Delta t_{pml}\) is greater than \(\Delta t_{cfl,1d}\) for any complex wavenumber.

### 3.6.2 Investigation for Two Dimensional Dispersion

![Figure 3.5: The structure of the PML [35]. The interior is vacuum.](image)

For the traveling waves to pass through the interior-PML interface without any reflections, the conductivities in the PML should be perfectly matched to the
conductivities in the interior region. By using only one pair of the conductivities \((\sigma_x \text{ and } \sigma_y^*)\) in the \(x\)-direction of the PML region while keeping the other conductivities \((\sigma_y \text{ and } \sigma_x^*)\) as the same as those in the interior field, and only using \(\sigma_y \text{ and } \sigma_x^*\) in the \(y\)-direction while \(\sigma_x \text{ and } \sigma_y^*\) are the same as the interior conductivities, the PML eliminates the interface reflection for any incidence angles and frequencies. Figure 3.5 shows that, the interior region of vacuum is surrounded by the CFS-PML and the total computational domain is bounded by PEC. The whole PML region is composed of four corners and four sides. The CFS-PML conductivities \(\sigma_x \text{ and } \sigma_x^*\) are set to zero in Region Top and Region Down, while \(\sigma_y \text{ and } \sigma_y^*\) are perfectly matched as \(\sigma_y \mu = \sigma_y^* \epsilon\). For CFS-PML in Region Left and Region Right, the conductivities are set to \((\sigma_x, \sigma_x^*, 0, 0)\). Note that, the four corners are overlapped by two adjacent CFS-PMLs, which have two pairs of the PML conductivities.

### 3.6.2.1 PML in the Four Corners

For the CFS-PML in the corners of the FDTD space, let us assume that \(\sigma_x = \sigma_y, \sigma_x^* = \sigma_y^*\) and \(\Delta x = \Delta y\). Then (3.72) is simplified to

\[
\left( e^{\frac{j \omega \Delta t}{2}} - a_x e^{-\frac{j \omega \Delta t}{2}} \right)^2 = \frac{(1 - a_x)^2 \epsilon^2_0}{\sigma_x^2 \Delta x^2} \left( e^{\frac{j \tilde{k}_x \Delta x}{2}} - e^{-\frac{j \tilde{k}_x \Delta x}{2}} \right)^2 + \frac{(1 - a_x)^2 \epsilon^2_0}{\sigma_y^2 \Delta y^2} \left( e^{\frac{j \tilde{k}_y \Delta y}{2}} - e^{-\frac{j \tilde{k}_y \Delta y}{2}} \right)^2
\]

(3.90)

where \(\tilde{k}_x = \frac{\omega}{c} \left( \kappa_x + \frac{\sigma_x}{\alpha_x + j \omega \epsilon_0} \right) \cos \varphi\) and \(\tilde{k}_y = \frac{\omega}{c} \left( \kappa_y + \frac{\sigma_y}{\alpha_y + j \omega \epsilon_0} \right) \sin \varphi\).

**The case of \(\varphi = 0, \pi/2, \pi\text{ and } 3\pi/2\)** With \(\alpha_x = \alpha_y\) and \(\kappa_x = \kappa_y\), if the wave is propagating along the major grid axes \((\varphi = 0, \pi/2, \pi\text{ and } 3\pi/2)\), (3.90) can be reduced to

\[
\frac{(1 - a_x)^2 \epsilon^2_0}{\sigma_x^2 \Delta x^2} \left( e^{\frac{j \frac{1}{2} \tilde{k}_x \Delta x}{2}} - e^{-\frac{j \frac{1}{2} \tilde{k}_x \Delta x}{2}} \right)^2 = \left( e^{\frac{j \frac{1}{2} \omega \Delta t}{2}} - a_x e^{-\frac{j \frac{1}{2} \omega \Delta t}{2}} \right)^2
\]

(3.91)
which is identical to the 1D PML dispersion equation in (3.53). Thus equations (3.83), (3.85) and (3.88) are the conditions for choosing the parameters of (3.91). In order to guarantee the stability in 2D computation, (3.85) and (3.88) have to be greater than $\Delta t_{cfl2d}$, which is the maximum $\Delta t$ under 2D CFL limit. With the parameters which are used to produce Figure 3.2, $\mathcal{Y}_A$ is displayed in Figure 3.6 and the comparison of $\Delta t_{pml}$ and $\Delta t_{cfl2d}$ is plotted in Figure 3.7. Since the results of $\Delta x = 2$ mm and $\Delta x = 0.5$ mm are identical to $\Delta x = 1$ mm, here we only show the variation of $\mathcal{Y}_A$ for the case of $\Delta x = 1$ mm in Figure 3.6. In Figure 3.6 and Figure 3.7, both (3.82) and (3.88) are satisfied for any complex wavenumber under the 2D CFL condition with the above parameters.

The case of $\varphi = \pi/4$, $3\pi/4$, $5\pi/4$ and $7\pi/4$ With $\alpha_x = \alpha_y$ and $\kappa_x = \kappa_y$, for the propagation angles of $\varphi = \pi/4$, $3\pi/4$, $5\pi/4$ and $7\pi/4$, the dispersion equation
Figure 3.7: The difference between $\Delta t_{pml}$ and $\Delta t_{cfl2d}$ varying $\frac{\Delta x\omega}{c}$ from zero to $\pi$ for the cases of $\Delta x = 2$ mm, $\Delta x = 1$ mm and $\Delta x = 0.5$ mm. $\Delta t_{cfl2d}$ is the upper limit of the 2D CFL condition.

(3.90) can be written as

$$
\left( e^{\frac{j\omega \Delta t}{2}} - a_x e^{-\frac{j\omega \Delta t}{2}} \right)^2 = 2 \left( 1 - a_x \right)^2 \frac{\epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( \frac{j \tilde{k}_x \Delta x}{2\sqrt{2}} - e^{-\frac{j \tilde{k}_x \Delta x}{2\sqrt{2}}} \right)^2 .
$$

(3.92)

Substituting Euler’s formulae and the complex wavenumber (3.73) into (3.92) yields

$$
\left( 1 - a_x \cos \left( \frac{\omega \Delta t}{2} \right) + j (1 + a_x) \sin \left( \frac{\omega \Delta t}{2} \right) \right)^2 =
$$

$$
\frac{2 (1 - a_x)^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( \Psi_1 - \Psi_1^{-1} \right) \cos \left( \frac{\Delta x \omega}{2\sqrt{2c}} A \right) + j (\Psi_1 + \Psi_1^{-1}) \sin \left( \frac{\Delta x \omega}{2\sqrt{2c}} A \right) \right)^2
$$

(3.93)

where

$$
\Psi_1 = e^{\frac{\Delta x \omega}{2\sqrt{2c}}} .
$$

(3.94)
consists of two parts. The real part is
\[
(1 + a_x^2)(2 \cos^2(\frac{\omega \Delta t}{2}) - 1) - 2a_x - \frac{2(1 - a_x)^2 c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi_1^2 + \Psi_1^{-2})(2 \cos^2(\frac{\Delta x \omega}{2\sqrt{2c}A}) - 1) - 2 \right) = 0
\] (3.95)
and the imaginary part is
\[
(1 - a_x^2) \sin(\omega \Delta t) = \frac{2(1 - a_x)^2 c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} (\Psi_1^2 - \Psi_1^{-2}) \sin(\frac{\Delta x \omega}{c\sqrt{2}}A).
\] (3.96)
Since \(0 \leq \cos^2(\frac{\omega \Delta t}{2}) \leq 1\), the real part (3.95) is written as
\[
0 \leq \frac{2(1 - a_x)^2 c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi_1^2 + \Psi_1^{-2})(2 \cos^2(\frac{\Delta x \omega}{2\sqrt{2c}A}) - 1) - 2 \right) + (1 + a_x)^2 \leq 2(1 + a_x^2)
\] (3.97)
which can be split to two inequalities. The first one is
\[
\mathcal{X}_B \triangleq \frac{2c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi_1^2 + \Psi_1^{-2}) \cos(\frac{\Delta x \omega}{c\sqrt{2}}A) - 2 \right) \leq 1
\] (3.98)
and the second one is
\[
0 \leq \left( \frac{1 - a_x}{1 + a_x} \right)^2 \frac{2c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left( (\Psi_1^2 + \Psi_1^{-2}) \cos(\frac{\Delta x \omega}{c\sqrt{2}}A) - 2 \right) + 1 \triangleq Y_B.
\] (3.99)
Since \(0 \leq \sin(\omega \Delta t) \leq 1\), \(\Psi_1^2 > \Psi_1^{-2}\) and \(0 < a_x < 1\), the imaginary part (3.96) is written as
\[
\frac{2c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} (\Psi_1^2 - \Psi_1^{-2}) \sin(\frac{\Delta x \omega}{c\sqrt{2}}A) \leq \frac{1 + a_x}{1 - a_x}.
\] (3.100)
Substituting (3.47) into (3.100), the condition for \(\Delta t\) is derived as
\[
\Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left( \frac{\frac{2c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} (\Psi_1^2 - \Psi_1^{-2}) \sin(\frac{\Delta x \omega}{c\sqrt{2}}A) + 1}{\frac{2c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} (\Psi_1^2 - \Psi_1^{-2}) \sin(\frac{\Delta x \omega}{c\sqrt{2}}A) - 1} \right) \triangleq \Delta t_{2d_{pml}}
\] (3.101)
where \(\frac{2c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} (\Psi_1^2 - \Psi_1^{-2}) \sin(\frac{\Delta x \omega}{c\sqrt{2}}A)\) should greater than one.
Let us define the left hand side of (3.98) as \(\mathcal{X}_B\), the right hand side of (3.99)
Figure 3.8: $\chi_B$ varying $\frac{\Delta x \omega}{c}$ from zero to $\pi$ for the cases of $\Delta x = 2$ mm, $\Delta x = 1$ mm and $\Delta x = 0.5$ mm.

as $Y_B$ and the right hand side of (3.101) as $\Delta t_{2dpml}$. The minimal $Y_B$ is obtained
at $\cos(\frac{\Delta x \omega}{c\sqrt{2}} A) = -1$. Then substituting (3.47) and $\frac{\Delta x \omega}{c\sqrt{2}} = \frac{\pi}{A}$ into (3.99) yields

$$
\Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left( \frac{\sqrt{2} \epsilon_0 \pi B}{\pi A} \left( e^{\frac{i B}{2\pi}} + e^{-\frac{i B}{2\pi}} \right) + 1 \right)
$$

where $\sqrt{\frac{\epsilon_0}{\sigma_x} A} (e^{\frac{i B}{2\pi}} + e^{-\frac{i B}{2\pi}})$ should be greater than one.

The conditions (3.98), (3.101) and (3.102) are stricter than (3.83), (3.85) and (3.88). Thus, for the CFS-PMLs in the four corners of the FDTD space, we should use conditions (3.98), (3.101) and (3.102) to choose the parameters. With
the CFS stretching coefficient which is used to produce Figure 3.2, Figure 3.8, 3.9 and 3.10 plot the the value of $\chi_B$, $Y_B$ and $\Delta t_{2dpml}$ over $\frac{\Delta x \omega}{c}$. The results in
Figure 3.8 all fulfill condition (3.98), which indicates that the parameters of the
CFS-PML can be used in both 1D and 2D calculations. The variation of $Y_B$ for
the case of $\Delta x = 1$ mm is displayed in Figure 3.6 The results of $Y_B$ in the cases
\[ \Delta t = \Delta t_{cfl} \]
\[ \Delta t = 0.8 \Delta t_{cfl} \]
\[ \Delta t = 0.5 \Delta t_{cfl} \]

\[ \nu_B \]

Figure 3.9: \( \nu_B \) varying \( \frac{\Delta x \omega}{c} \) from zero to \( \pi \) for the case of \( \Delta x = 1 \) mm. \( \Delta t_{cfl} \) is the upper limit of the 2D CFL condition for \( \Delta t \).

of \( \Delta x = 2 \) mm and \( \Delta x = 0.5 \) mm are identical to \( \Delta x = 1 \) mm. Figures 3.9 and 3.10 show that, conditions (3.99) and (3.101) are satisfied for any complex wavenumber with the above parameters.

### 3.6.2.2 PML in the Four Sides

As shown in Figure 3.5, the conductivity is set to \((\sigma_x, \sigma_x^*, 0, 0)\) for the CFS-PML in Region_Left and Region_Right, and \((0, 0, \sigma_y, \sigma_y^*)\) in Region_Top and Region_Down. If \( \sigma_x = \sigma_y, \kappa_x = \kappa_y, \alpha_x = \alpha_y \) and \( \Delta x = \Delta y \), the dispersion relations in the left and right sides are identical to the top and bottom. For the CFS-PML in Region_Left and Region_Right, when we assume that \( \sigma_x = \sigma_y \) and \( \Delta x = \Delta y \), the numerical dispersion (3.72) is simplified to

\[
\left( \frac{1 - \alpha_x}{\sigma_x^2} \right)^2 c^2 \frac{\epsilon_0^2}{\Delta x^2} \left( e^{j \frac{1}{2} k_x \Delta x} - e^{-j \frac{1}{2} k_x \Delta x} \right)^2 \left( e^{j \frac{1}{2} \omega \Delta t} - e^{-j \frac{1}{2} \omega \Delta t} \right)^2 \\
+ c^2 \frac{\Delta t^2}{\Delta x^2} \left( e^{j \frac{1}{2} k_x \Delta x} - e^{-j \frac{1}{2} k_x \Delta x} \right)^2 \left( e^{j \frac{1}{2} \omega \Delta t - \alpha_x e^{-j \frac{1}{2} \omega \Delta t}} \right)^2 \\
= \left( e^{j \frac{1}{2} \omega \Delta t - \alpha_x e^{-j \frac{1}{2} \omega \Delta t}} \right)^2 \left( e^{j \frac{1}{2} \omega \Delta t - e^{-j \frac{1}{2} \omega \Delta t}} \right)^2 
\] (3.103)
\[
\frac{(\Delta t_{2dpm}/\Delta t_{cfl})^2}{\Delta x} - 1 \geq 0.5 \text{mm} \\
\Delta x = 1 \text{mm} \\
\Delta x = 0.5 \text{mm}
\]

Figure 3.10: The difference between \(\Delta t_{2dpm}\) and \(\Delta t_{cfl}\) varying \(\frac{\Delta x \omega}{c}\) from zero to \(\pi\) for the cases of \(\Delta x = 2\) mm, \(\Delta x = 1\) mm and \(\Delta x = 0.5\) mm. \(\Delta t_{cfl}\) is the upper limit of the 2D CFL condition for \(\Delta t\).

where \(\tilde{k}_x = \frac{\omega}{c}\left(\kappa_x + \frac{\sigma_x}{\alpha_x + j\omega}\right)\cos \varphi\) and \(\tilde{k}_y = \frac{\omega}{c}\kappa_y \sin \varphi\).

**The case of \(\varphi = 0\) and \(\pi\)** If the wave is propagating along the \(x\)-axis (\(\varphi = 0\) and \(\pi\)), the wavenumber in the \(y\)-direction is zero (\(\tilde{k}_y = 0\)). In this case, \((3.103)\) is reduced to \((3.91)\). Therefore the conditions \((3.83)\), \((3.85)\) and \((3.88)\) can be used to choose the parameters for the propagation angles of \(\varphi = 0\) and \(\pi\) in Region\_Left and Region\_Right.

**The case of \(\varphi = \pi/2\) and \(3\pi/2\)** If the wave is propagating in the \(y\)-direction (\(\varphi = \pi/2\) and \(3\pi/2\)), we obtain that \(\tilde{k}_x = 0\) and \(\tilde{k}_y = \frac{\omega}{c}\kappa_y\). Then \((3.103)\) is reduced to

\[
\frac{c^2 \Delta t^2}{\Delta x^2} \left( e^{j\frac{1}{2}\kappa_y \Delta x} - e^{-j\frac{1}{2}\kappa_y \Delta x} \right)^2 = \left( e^{j\frac{1}{2}\omega \Delta t} - e^{-j\frac{1}{2}\omega \Delta t} \right)^2
\]

\[
\therefore \frac{c^2 \Delta t^2}{\Delta x^2} \sin^2 \left( \frac{1}{2} \frac{\omega}{c} \kappa_y \Delta x \right) = \sin^2 \left( \frac{1}{2} \frac{\omega}{c} \Delta t \right).
\]

\(3.104\)

Since \(0 \leq \sin^2 \left( \frac{1}{2} \frac{\omega}{c} \Delta t \right) \leq 1\), we can derive that \(0 \leq \frac{c^2 \Delta t^2}{\Delta x^2} \sin \left( \frac{1}{2} \frac{\omega}{c} \kappa_y \Delta x \right)^2 \leq 1\).
The maximal value of \( \sin(\frac{1}{2}c_\kappa \Delta x) \) is one, thus \( \Delta t \leq \frac{\Delta x}{c} \), which is the same as the CFL condition. In summary, in the four sides of the PML and the propagation angles of \( \varphi = 0, \pi/2, \pi \) and \( 3\pi/2 \), the computation is stable with the \( \Delta t \), which is chosen under the CFL condition and the conditions (3.83), (3.85) and (3.88).

The case of \( \varphi = \pi/4, 3\pi/4, 5\pi/4 \) and \( 7\pi/4 \) Let us assume that \( \kappa_x = \kappa_y \), for the wave is propagating along the diagonals of the grid (\( \varphi = \pi/4, 3\pi/4, 5\pi/4 \) and \( 7\pi/4 \)) in Region Left and Region Right, the wavenumbers are manipulated as \( \hat{k}_x = \frac{\omega}{\sqrt{2}c} (\kappa_x + \frac{\sigma_x}{\alpha_x + j\omega_0}) \) and \( \hat{k}_y = \frac{\omega}{\sqrt{2}c} \kappa_x \). Then (3.103) is reduced to

\[
(1-a_x)^2 \epsilon_0^2 \left( e^{\frac{\Delta x \omega \kappa}{2 c}} A - e^{-\frac{\Delta x \omega \kappa}{2 c}} A e^{-\frac{\Delta x \omega \kappa}{2 c}} B \right)^2 \left( e^{\frac{\Delta t}{2} \omega} - e^{-\frac{\Delta t}{2} \omega} \right)^2
\]

\[
+ \frac{c^2 \Delta t^2}{\Delta x^2} \sin^2(\frac{\kappa_x \omega \Delta x}{2\sqrt{2}c}) \left( (1 + a_x^2)(1 - 2 \sin^2(\frac{\omega \Delta t}{2})) - 2a_x + j(1 - a_x^2) \sin(\omega \Delta t) \right)
\]

\[
= \left( (1 + a_x^2)(1 - 2 \sin^2(\frac{\omega \Delta t}{2})) - 2a_x + j(1 - a_x^2) \sin(\omega \Delta t) \right) \sin^2(\frac{\omega \Delta t}{2})
\]

(3.106)

Substituting Euler’s formulae into (3.105) yields

\[
(1-a_x)^2 \epsilon_0^2 \left( e^{\frac{\Delta x \omega \kappa}{2 c}} A - e^{-\frac{\Delta x \omega \kappa}{2 c}} A e^{-\frac{\Delta x \omega \kappa}{2 c}} B \right)^2 \left( e^{\frac{\Delta t}{2} \omega} - e^{-\frac{\Delta t}{2} \omega} \right)^2
\]

\[
+ \frac{c^2 \Delta t^2}{\Delta x^2} \sin^2(\frac{\kappa_x \omega \Delta x}{2\sqrt{2}c}) \left( (1 + a_x^2)(1 - 2 \sin^2(\frac{\omega \Delta t}{2})) - 2a_x + j(1 - a_x^2) \sin(\omega \Delta t) \right)
\]

\[
= \left( (1 + a_x^2)(1 - 2 \sin^2(\frac{\omega \Delta t}{2})) - 2a_x + j(1 - a_x^2) \sin(\omega \Delta t) \right) \sin^2(\frac{\omega \Delta t}{2})
\]

(3.106)

where

\[
\mathcal{F}_A = (\Psi_1^2 + \Psi_1^{-2}) \cos(\frac{\Delta x \omega}{\sqrt{2}c} A) - 2
\]

(3.107)

and

\[
\mathcal{F}_B = (\Psi_1^2 - \Psi_1^{-2}) \sin(\frac{\Delta x \omega}{\sqrt{2}c} A).
\]

(3.108)
(3.106) can be separated into two parts. The real part is

\[
\frac{(1-a_x)^2 c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \sin^2\left(\frac{\omega \Delta t}{2}\right) \mathcal{F}_A + \frac{c^2 \Delta t^2}{\Delta x^2} \sin^2\left(\frac{\kappa y \omega \Delta x}{2\sqrt{2}c}\right) \left(1 - a_x^2 \right) - 2\left(1 + a_x^2\right) \sin^2\left(\frac{\omega \Delta t}{2}\right) = \left(1 - a_x^2 \right) - 2\left(1 + a_x^2\right) \sin^2\left(\frac{\omega \Delta t}{2}\right)
\]

and the imaginary part is

\[
\frac{(1-a_x)^2 c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \sin^2\left(\frac{\omega \Delta t}{2}\right) \mathcal{F}_B + \frac{c^2 \Delta t^2}{\Delta x^2} \sin^2\left(\frac{\kappa y \omega \Delta x}{2\sqrt{2}c}\right) \left(1 - a_x^2\right) \sin(\omega \Delta t) - (1 - a_x^2) \sin (\omega \Delta t) \sin^2\left(\frac{\omega \Delta t}{2}\right) = 0.
\]

Let us manipulate the real part equation (3.109) as

\[
\frac{(1-a_x)^2 c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \sin^2\left(\frac{\omega \Delta t}{2}\right) \mathcal{F}_A + \frac{c^2 \Delta t^2}{\Delta x^2} \sin^2\left(\frac{\kappa y \omega \Delta x}{2\sqrt{2}c}\right) \left(1 - a_x^2\right) \sin(\omega \Delta t)
\]

\[
+ 2\left(1 + a_x^2\right) \sin^4\left(\frac{\omega \Delta t}{2}\right) + \mathcal{Z}_{A1} \sin^2\left(\frac{\omega \Delta t}{2}\right) + \mathcal{Z}_{A2} = 0.
\]

Since \(2(1 + a_x^2)\) is a positive value, (3.111) can be written as

\[
\sin^4\left(\frac{\omega \Delta t}{2}\right) + \mathcal{Z}_{A1} \sin^2\left(\frac{\omega \Delta t}{2}\right) + \mathcal{Z}_{A2} = 0
\]

where

\[
\mathcal{Z}_{A1} = \frac{(1-a_x)^2 c^2 \epsilon_0^2}{2(1 + a_x^2)\sigma_x^2 \Delta x^2} \mathcal{F}_A - \frac{(1-a_x)^2}{2(1 + a_x^2)} - \frac{c^2 \Delta t^2}{\Delta x^2} \sin^2\left(\frac{\kappa y \omega \Delta x}{2\sqrt{2}c}\right)
\]

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and

\[ Z_{A2} = \frac{c^2 \Delta t^2}{2 \Delta x^2} \sin^2 \left( \frac{\kappa \omega \Delta x}{2 \sqrt{2c}} \right) \left( \frac{1 - a_x}{1 + a_x^2} \right)^2. \]  

(3.114)

If \( Z_{A1}^2 - 4Z_{A2} < 0 \), the left hand side of (3.112) is greater than zero for any real \( \omega \), which is instable for any \( \Delta t \). For \( Z_{A1}^2 - 4Z_{A2} \geq 0 \), let us write (3.112) as

\[
\left( \sin^2 \left( \frac{\omega \Delta t}{2} \right) + \frac{Z_{A1} - \sqrt{Z_{A1}^2 - 4Z_{A2}}}{2} \right) \left( \sin^2 \left( \frac{\omega \Delta t}{2} \right) + \frac{Z_{A1} + \sqrt{Z_{A1}^2 - 4Z_{A2}}}{2} \right) = 0
\]

(3.115)

which can be separated into two equations of

\[
\sin^2 \left( \frac{\omega \Delta t}{2} \right) + \frac{Z_{A1} - \sqrt{Z_{A1}^2 - 4Z_{A2}}}{2} = 0
\]

(3.116)

and

\[
\sin^2 \left( \frac{\omega \Delta t}{2} \right) + \frac{Z_{A1} + \sqrt{Z_{A1}^2 - 4Z_{A2}}}{2} = 0
\]

(3.117)

Since \( 0 \leq \sin^2 \left( \frac{\omega \Delta t}{2} \right) \leq 1 \), (3.116) and (3.117) can be written as

\[
0 \leq -Z_{A1} + \sqrt{Z_{A1}^2 - 4Z_{A2}} \leq 1
\]

(3.118)

and

\[
0 \leq -Z_{A1} - \sqrt{Z_{A1}^2 - 4Z_{A2}} \leq 1
\]

(3.119)

When \( Z_{A1} \geq 0 \), \((-Z_{A1} + \sqrt{Z_{A1}^2 - 4Z_{A2}})\) and \((-Z_{A1} - \sqrt{Z_{A1}^2 - 4Z_{A2}})\) are equal to or smaller than zero due to \( Z_{A2} \geq 0 \). \((-Z_{A1} + \sqrt{Z_{A1}^2 - 4Z_{A2}})\) equals zero when \( Z_{A2} = 0 \). \((-Z_{A1} - \sqrt{Z_{A1}^2 - 4Z_{A2}})\) equals zero when \( Z_{A1} = Z_{A2} = 0 \). However, \( Z_{A2} \) equals zero only at \( \frac{\omega \Delta x}{c} = 0 \). Therefore, for \( Z_{A1} \geq 0 \), (3.115) is not satisfied for any real \( \frac{\omega \Delta x}{c} \), which may cause numerical instability.

When \( Z_{A1} < 0 \), \((-Z_{A1} + \sqrt{Z_{A1}^2 - 4Z_{A2}})\) and \((-Z_{A1} - \sqrt{Z_{A1}^2 - 4Z_{A2}})\) is alway equal to or greater than zero due to \( Z_{A2} \geq 0 \). Thus (3.118) and (3.119)
can be simplified to

\[-\sqrt{Z_{A_1}^2 - 4Z_{A_2}} \leq 2 + Z_{A_1}\]  

(3.120)

and

\[\sqrt{Z_{A_1}^2 - 4Z_{A_2}} \leq 2 + Z_{A_1}.\]  

(3.121)

(3.115) is valid when either (3.120) or (3.121) is satisfied.

Consequently, the parameters in (3.111) can be chosen based on the following conditions: 

\[Z_{A_1}^2 - 4Z_{A_2} \geq 0, \quad Z_{A_1} < 0 \quad \text{and} \quad -\sqrt{Z_{A_1}^2 - 4Z_{A_2}} \leq 2 + Z_{A_1} \quad \text{and} \quad \sqrt{Z_{A_1}^2 - 4Z_{A_2}} \leq 2 + Z_{A_1}.\]

In the range of \(0 \leq \omega \Delta t \leq \pi\), \(\sin^2\left(\frac{\omega \Delta t}{2}\right)\) equals zero only at \(\omega \Delta t = 0\). When \(\sin^2\left(\frac{\omega \Delta t}{2}\right) = 0\), the left hand side of (3.109) equal zero since \(\omega \Delta t = 0\). Thus the imaginary part equation (3.109) is valid for any \(\Delta t\) if \(\sin^2\left(\frac{\omega \Delta t}{2}\right) = 0\).

### 3.7 Summary

After reviewing the conception of numerical dispersion and stability of the FDTD method, this chapter presented the dispersion relation and stability condition of the CFS-PML in Sections 3.5 and 3.6. Section 3.5 introduced the numerical dispersion relation for the CFS-PML by discretizing Maxwell’s curl equations with exponential difference. Based on the derived dispersion relation in Section 3.5, Section 3.6 derived the stability conditions of the CFS-PML in both 1D and 2D scenarios. In the 1D computation, the parameters of the CFS-PML should satisfy condition in (3.81) and the temporal increment should satisfy conditions in (3.85) and (3.88). In the 2D case, (3.98) is the condition for setting parameters of the CFS-PML and (3.101) and (3.102) are the conditions for determining the time discretization of the CFS-PML.
Chapter 4

Spatial Filtering Approach

The numerical dispersion is a non-physical characteristic of the FDTD method that constrains the spatial and temporal size to guarantee the accuracy and stability. For the simulations with electrically small objects or dispersive materials, the spatio-temporal resolution is required to be high, which costs massive memory and long execution time. To improve the computational speed, the implicit schemes are developed for extending the CFL limit unconditionally. However, these schemes generate undesirable errors when the temporal interval is increased. As an alternative to these implicit schemes, the spatial filtering approach removes the spurious frequency components in the electromagnetic fields to gain large temporal interval \[13\] \[14\] \[60\]. This chapter describes the principle of the spatial filtering approach and shows the procedures of this approach.

4.1 Implicit FDTD Methods

The conventional explicit FDTD method, which is computationally simple and numerically accurate, updates the electromagnetic fields with the information at the previous time steps. However, due to the CFL condition, the maximum temporal discretization of the explicit FDTD method depends on the spatial discretization. The implicit schemes, such as the alternating direction implicit FDTD (ADI-FDTD) method \[61\] \[62\] \[63\], Crank-Nicolson FDTD (CN-FDTD) method \[64\] and locally one dimensional FDTD (LOD-FDTD) method \[65\], are developed to relax or overcome the CFL condition. These implicit schemes reformulate the conventional Yee algorithm and update the electric and magnetic fields simultaneously at each time steps. In the implicit FDTD methods, the
maximum temporal discretization is independent of the spatial discretization.

To exceed the CFL limit unconditionally, the Crank-Nicolson (CN) scheme is applied to Maxwell’s equations in order to reformulate the conventional FDTD method [66][67]. The irreducible heavy matrix computation restrains the further application of the CN-FDTD method, although the CN-FDTD method presents the potential of giving high accuracy computation and small numerical dispersion error [68]. The ADI-FDTD, Douglas-Gunn FDTD and split-step FDTD methods are developed to reduce the computational complexity of the CN-FDTD method [64][69][70]. However these methods generate additional numerical errors.

The numerical approximation of the ADI-FDTD method is second order accurate in both time and space. The accuracy of the solution is only first order accurate in the first sub-step, but rises to second order accurate following the second sub-step [64]. If $\Delta t$ is less than the upper limit of the CFL condition, the numerical dispersion error of the ADI-FDTD method is similar to the conventional FDTD method. However, if $\Delta t$ exceeds the CFL limit, the numerical dispersion of the ADI-FDTD method increases while $\Delta t$ enlarges [71][72]. Therefore, although the ADI-FDTD method is unconditionally stable, the choice of $\Delta t$ is dependent on the desired accuracy.

Apart from the high dispersion error with large $\Delta t$, the accuracy of the ADI-FDTD method is also affected by its explicit source excitation [73][74]. Mathematically, the ADI-FDTD method is a simplification of the CN-FDTD method, and can be regarded as an $O(\Delta t^2)$ perturbation of the CN-FDTD method [72]. Reported by Jun Shibayama [65], the LOD-FDTD method only has a splitting error of $O(\Delta t)$ by comparing to the CN-FDTD method [75]. The three dimensional LOD-FDTD method discretizes Maxwell’s equation with Crank-Nicolson approximation and splits a single time step to three sub-steps [76]. Each sub-step solves electromagnetic field components in one direction. The recursive equations of each direction are independent of the other directions, which can be solved by a linear tridiagonal system. Thus, comparing to the ADI-FDTD method, the LOD-FDTD method is simpler in implementation and more efficient in computation [76].

To summarize, the implicit FDTD methods are unconditionally stable, but increase the computational complexity of the conventional FDTD and sacrifice the accuracy to exceed the CFL condition.
4.2 Idea of the Spatial Filtering Approach

In high accuracy computations, the fine spatial sampling provides a wide bandwidth in the spatial frequency domain. However, the excited signal only engages a small part of the bandwidth. The remaining part of the bandwidth contains no signal information, but increases the numerical dispersion which restrains the temporal size for stable computations. In contrast with the implicit schemes, instead of reformulating the time marching equations of the conventional FDTD method, the spatial filtering approach extends the CFL limit by removing the unstable harmonics in the high spatial frequency range \[13\] \[14\]. This approach is conditionally stable since the bandwidth with signals still carries spurious frequency components that cause numerical dispersion.

4.2.1 Revised 1D CFL Condition

For any real \( \omega \), the sinusoidal term \( \sin\left(\frac{k_0 \Delta x}{2}\right) \) of (3.27) is always smaller than one. Thus (3.27) can be written as

\[
\frac{c \Delta t}{\Delta x} \sin\left(\frac{k_0 \Delta x}{2}\right) \leq 1.
\] (4.1)

Based on (4.1), the condition for \( \Delta t \) is expressed as

\[
\Delta t \leq \frac{\Delta x}{c} \frac{1}{\sin\left(\frac{k_0 \Delta x}{2}\right)}.
\] (4.2)

To guarantee the stability, \( \Delta t \) should be smaller than the minimum value of the right hand side of (4.2). Since the maximum value of \( \sin\left(\frac{k_0 \Delta x}{2}\right) \) is one for any real wavenumber, the upper limit of \( \Delta t \) for stable computation is \( \frac{\Delta x}{c} \), which is the 1D CFL limit. For the purpose of decreasing the numerical dispersion, \( \Delta x \) should be shorter than one-tenth of \( \lambda_{\text{min}} \). If \( \Delta x = \frac{\lambda_{\text{min}}}{10} \), the highest wavenumber of the excited signal is \( \tilde{k}_{\text{highest}} = \frac{2\pi}{\lambda_{\text{min}}} = \frac{\pi}{5 \Delta x} \). However, according to the Nyquist sampling theorem, the maximum spatial frequency in the FDTD computation is \( \frac{1}{2\Delta x} \), thus the greatest wavenumber that the FDTD method can accommodate is \( \tilde{k}_0 = 2\pi \frac{1}{2\Delta x} = \frac{\pi}{\Delta x} \). Therefore the wavenumbers from \( \frac{\pi}{5 \Delta x} \) to \( \frac{\pi}{\Delta x} \) do not carry source excitations but generate undesired dispersion errors. By filtering out these spurious frequency components, we can extend the CFL condition conditionally.
The revised CFL condition is defined as
\[
\Delta t \leq \frac{\Delta x}{c} \frac{1}{\sin \left( \frac{k_{\text{max}} \Delta x}{2} \right)}
\]  
(4.3)

where \( k_{\text{max}} \) is the filtering wavenumber and the spatial frequency components in the range of \( k_{\text{max}} < k \leq \frac{\pi}{\Delta x} \) are filtered out [13]. The upper limit of (4.3) is greater than the upper limit of the 1D CFL condition (\( \frac{\Delta x}{c} \)) with a factor of \( \frac{1}{\sin \left( \frac{k_{\text{max}} \Delta x}{2} \right)} \).

4.2.2 Revised 2D CFL Condition

To satisfy any real \( \omega \) (\( \sin \left( \frac{\Delta \omega}{2} \right) \leq 1 \)), the 2D numerical dispersion (3.26) can be written as
\[
\Delta t \leq \frac{1}{c \sqrt{\sin^2 \left( \frac{k \cos \phi \Delta x}{2} \right) + \sin^2 \left( \frac{k \sin \phi \Delta y}{2} \right)}}.
\]  
(4.4)

If \( \Delta x = \Delta y \), by filtering out the wavenumbers higher than \( k_{\text{max}} \) in (4.4), the revised 2D CFL condition for \( \Delta t \) is obtained as
\[
\Delta t \leq \frac{\Delta x}{c} \frac{1}{\sqrt{\sin^2 \left( \frac{k_{\text{max}} \cos \phi \Delta x}{2} \right) + \sin^2 \left( \frac{k_{\text{max}} \sin \phi \Delta x}{2} \right)}}.
\]  
(4.5)

Let us define \( \frac{1}{\sqrt{\sin^2 \left( \frac{k_{\text{max}} \Delta x \cos \phi}{2} \right) + \sin^2 \left( \frac{k_{\text{max}} \Delta x \sin \phi}{2} \right)} } \) as \( K_A(\phi) \). According to the Nyquist sampling theorem, \( k_{\text{max}} \Delta x \) can take any value from zero to \( \pi \). Figures 4.1 plots the variation of \( K_A(\phi) \) for the cases of \( k_{\text{max}} \Delta x = \pi, \frac{\pi}{2}, \text{ and } \frac{\pi}{4} \), which shows that the minimum value of \( K_A(\phi) \) occurs at \( \phi = \frac{\pi}{4} \) and \( \frac{3\pi}{4} \). In the range of \( 0 \leq \phi \leq \pi \), the first derivative of \( K_A(\phi) \) with respect to \( \phi \) equals zero at \( \phi = 0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}, \text{ and } \pi \). Substituting the above five angles into the second derivative of \( K_A(\phi) \) with respect to \( \phi \), \( K_A(\phi)'' \) is positive at \( \phi = \frac{\pi}{4} \) and \( \frac{3\pi}{4} \). Therefore the minimum value of \( K_A(\phi) \) takes place at \( \phi = \frac{\pi}{4} \) and \( \frac{3\pi}{4} \), which are the angles at...
\[ \tilde{k}_{\text{max}} \Delta x = \pi \]
\[ \tilde{k}_{\text{max}} \Delta x = \frac{\pi}{2} \]
\[ \tilde{k}_{\text{max}} \Delta x = \frac{\pi}{4} \]

Figure 4.1: \( K_A \) varying \( \varphi \) from zero to \( \pi \) for the cases of \( \tilde{k}_{\text{max}} \Delta x = \pi \), \( \tilde{k}_{\text{max}} \Delta x = \frac{\pi}{2} \) and \( \tilde{k}_{\text{max}} \Delta x = \frac{\pi}{4} \).

the diagonals of a 2D cell. Substituting \( \varphi = \frac{\pi}{4} \) and \( \frac{3\pi}{4} \) into (4.5) yields

\[ \Delta t \leq \frac{\Delta x}{c \sqrt{2} \sin \left( \frac{\tilde{k}_{\text{max}} \Delta x}{2 \sqrt{2}} \right)} \]

which is the revised 2D CFL condition for any propagation angle \([14]\). The upper limit of (4.6) is greater than the upper limit of the conventional 2D CFL condition \( \left( \frac{\Delta x}{c \sqrt{2}} \right) \) with a factor of \( 1/ \sin \left( \frac{\tilde{k}_{\text{max}} \Delta x}{2 \sqrt{2}} \right) \).

4.3 Revised Stability Condition for CFS-PML

4.3.1 Revised Stability Condition for 1D CFS-PML

(3.85) and (3.88) are the two conditions that define the upper bound of \( \Delta t \) for stable computation in the CFS-PML. The revised stability condition of (3.85) is derived from (3.82). First, let us write (3.82) as

\[ \left( 1 - a_x \right)^2 \left( \frac{c^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \right) \left( 2 - (\Psi^2 + \Psi^{-2}) \cos \left( \frac{\Delta x \omega A}{c} \right) \right) \leq 1. \]
If \((\Psi^2 + \Psi^{-2}) \cos(\frac{\Delta x \omega}{c} A)\) is equal to or greater than two, the left hand side of (4.7) is always smaller than zero, which is stable for any \(\Delta t\). If \((\Psi^2 + \Psi^{-2}) \cos(\frac{\Delta x \omega}{c} A)\) is smaller than two, (4.7) can be written as

\[
\left(1 - \frac{a_x}{1 + a_x}\right)^2 \leq \frac{1}{\sigma_x^2 \Delta x^2} \left(2 - \left(\Psi^2 + \Psi^{-2}\right) \cos(\frac{\Delta x \omega}{c} A)\right).
\] (4.8)

Substituting (3.47) into (4.8) yields

\[
\left(1 - e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}\right)^2 \leq \frac{1}{\sigma_x^2 \Delta x^2} \left(2 - \left(\Psi^2 + \Psi^{-2}\right) \cos(\frac{\Delta x \omega}{c} A)\right).
\] (4.9)

Since \(0 < e^{-\frac{\sigma_x \Delta t}{\epsilon_0}} < 1\), (4.10) can be simplified to

\[
\frac{1 - e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}}{1 + e^{-\frac{\sigma_x \Delta t}{\epsilon_0}}} \leq \frac{1}{\sigma_x^2 \Delta x^2 \sqrt{\left(2 - \left(\Psi^2 + \Psi^{-2}\right) \cos(\frac{\Delta x \omega}{c} A)\right)}}.
\] (4.10)

With the similar derivation in (3.85), (4.10) can be manipulated as

\[
\Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left(\frac{\frac{\sigma_x \Delta x}{\epsilon_0} \sqrt{\left(2 - \left(\Psi^2 + \Psi^{-2}\right) \cos(\frac{\Delta x \omega}{c} A)\right) + 1}}{\frac{\sigma_x \Delta x}{\epsilon_0} \sqrt{\left(2 - \left(\Psi^2 + \Psi^{-2}\right) \cos(\frac{\Delta x \omega}{c} A)\right) - 1}}\right).
\] (4.11)

where \(\frac{\sigma_x \Delta x}{\epsilon_0} \sqrt{\left(2 - \left(\Psi^2 + \Psi^{-2}\right) \cos(\frac{\Delta x \omega}{c} A)\right)}\) should be greater than one. Based on (3.73) and (3.75), the 1D numerical wavenumber is written as

\[
\tilde{k}_x = \frac{\omega}{c} (A + jB).
\] (4.12)

In the numerical calculations, \(0 \leq \frac{\omega}{c} \leq \tilde{k}_0 = \frac{\pi}{\Delta x}\). Thus, when we filter out the wavenumbers from \(\tilde{k}_{max}\) to \(\tilde{k}_0\), (4.11) can be written as

\[
\Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left(\frac{\frac{\sigma_x \Delta x}{\epsilon_0} \sqrt{\left(2 - \left(e^{\Delta x \tilde{k}_{max} B} + e^{-\Delta x \tilde{k}_{max} B}\right) \cos(\Delta x \tilde{k}_{max} A)\right) + 1}}{\frac{\sigma_x \Delta x}{\epsilon_0} \sqrt{\left(2 - \left(e^{\Delta x \tilde{k}_{max} B} + e^{-\Delta x \tilde{k}_{max} B}\right) \cos(\Delta x \tilde{k}_{max} A)\right) - 1}}\right).
\] (4.13)
\[ \Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left( \frac{e^{c_x^2 \frac{\Delta x}{\sigma_x^2}} (e^{\Delta x \tilde{k}_{\max} B} - e^{-\Delta x \tilde{k}_{\max} B}) \sin(\Delta x \tilde{k}_{\max} A) + 1}{e^{c_x^2 \frac{\Delta x}{\sigma_x^2}} (e^{\Delta x \tilde{k}_{\max} B} - e^{-\Delta x \tilde{k}_{\max} B}) \sin(\Delta x \tilde{k}_{\max} A) - 1} \right). \quad (4.14) \]

(4.13) and (4.14) are the two revised stability conditions for the filtered FDTD method with CFS-PML in 1D. Let us define the upper limit of \( \Delta t \) in (4.3) as \( K_C \), in (4.13) as \( K_D \) and in (4.14) as \( K_E \). With the same \( \sigma_x \), \( \kappa_x \) and \( \alpha_x \) used in Figure 3.2, Figures 4.2 and 4.3 show the variation of \( K_C \), \( K_D \) and \( K_E \) with respect to \( \tilde{k}_{\max} \Delta x \). For the same \( \Delta x \), the curve of \( K_D \) is identical to \( K_C \) in Figure 4.2. In Figure 4.3 for the case of \( \Delta x = 2 \) mm, \( K_E \) is always greater than \( K_C \) with the same filtering wavenumber \( \tilde{k}_{\max} \). However \( K_E \) is smaller than \( K_C \) in the range of \( \frac{\pi}{2} \times \tilde{k}_{\max} \Delta x < \frac{2\pi}{5} \) when \( \Delta x = 1 \) mm. In the case of \( \Delta x = 0.5 \) mm, \( K_E \) is smaller than \( K_C \) in the range of \( \frac{2\pi}{5} \times \tilde{k}_{\max} \Delta x < \frac{2\pi}{3} \). Thus, we should set \( \Delta t \) based on both (4.13) and (4.14).
Figure 4.3: The value of $K_C$, $K_E$ varying $\tilde{k}_{max} \Delta x$ from zero to $\pi$ for the cases of $\Delta x = 2$ mm, 1 mm and 0.5 mm.
\[ \Delta x = 2 \text{ mm, } K_G \quad \Delta x = 2 \text{ mm, } K_F \]
\[ \Delta x = 1 \text{ mm, } K_G \quad \Delta x = 1 \text{ mm, } K_F \]
\[ \Delta x = 0.5 \text{ mm, } K_G \quad \Delta x = 0.5 \text{ mm, } K_F \]

Figure 4.4: The value of $K_F$ and $K_G$ varying $\tilde{k}_{\text{max}} \Delta x$ from zero to $\pi$ for the cases of $\Delta x = 2$ mm, 1 mm and 0.5 mm.

### 4.3.2 Revised Stability Condition for 2D CFS-PML

For the CFS-PML in the four corners of the 2D FDTD space, the stability conditions are given by (3.101) and (3.102). The revised stability of (3.102) is derived from (3.99). If $(\Psi_1^2 + \Psi_1^{-2}) \cos(\frac{\Delta x \omega}{c\sqrt{2}} A)$ is equal to or greater than two, the right hand side of (3.99) is always greater than zero, which is stable for any $\Delta t$. If $(\Psi_1^2 + \Psi_1^{-2}) \cos(\frac{\Delta x \omega}{c\sqrt{2}} A)$ is smaller than two, (3.99) can be written as

\[
\left( \frac{1 - a_x}{1 + a_x} \right)^2 \leq \frac{1}{2c^2 \sigma_x^2 \Delta x^2 \left( 2 - (\Psi_1^2 + \Psi_1^{-2}) \cos(\frac{\Delta x \omega}{c\sqrt{2}} A) \right)}. \tag{4.15}
\]

Substituting (3.47) into (4.15), the condition for $\Delta t$ is derived as

\[
\Delta t \leq \frac{\varepsilon_0}{\sigma_x} \ln \left( \frac{\sqrt{\varepsilon_0 \sigma_x}}{\varepsilon_0 \Delta x} \sqrt{ \left( 2 - (\Psi_1^2 + \Psi_1^{-2}) \cos(\frac{\Delta x \omega}{c\sqrt{2}} A) \right) + 1 } - 1 \right) \tag{4.16}
\]
Figure 4.5: The value of $K_F$, $K_H$ varying $\tilde{k}_{max}\Delta x$ from zero to $\pi$ for the cases of $\Delta x = 2$ mm, 1 mm and 0.5 mm.
where $\sqrt{2}c_0\Delta x \sqrt{\left(2 - (\Psi_1^2 + \Psi_1^{-2}) \cos\left(\frac{\Delta x \omega}{\sqrt{2}} A\right)\right)}$ should be greater than one. Filtering out the wavenumbers higher than $\tilde{k}_{\text{max}}$, (4.16) is written as

$$\Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left(\frac{\sqrt{2}c_0}{\sigma_x \Delta x} \sqrt{\left(2 - \left(e^{\frac{\Delta x \tilde{k}_{\text{max}} B}{\sqrt{2}}} + e^{-\frac{\Delta x \tilde{k}_{\text{max}} B}{\sqrt{2}}} \right) \cos\left(\frac{\Delta x \tilde{k}_{\text{max}}}{\sqrt{2}} A\right) + 1\right)} - 1\right)$$

and (3.101) is written as

$$\Delta t \leq \frac{\epsilon_0}{\sigma_x} \ln \left(\frac{2c_0^2 \epsilon_0^2}{\sigma_x^2 \Delta x^2} \left(e^{\frac{\Delta x \tilde{k}_{\text{max}} B}{\sqrt{2}}} - e^{-\frac{\Delta x \tilde{k}_{\text{max}} B}{\sqrt{2}}} \right) \sin\left(\frac{\Delta x \tilde{k}_{\text{max}}}{\sqrt{2}} A\right) + 1\right) \sin\left(\frac{\Delta x \tilde{k}_{\text{max}}}{\sqrt{2}} A\right) - 1\right).$$

Let us define the upper limit of $\Delta t$ in (4.6) as $K_F$, in (4.17) as $K_G$ and in (4.18) as $K_H$. Figures 4.4 and 4.5 plot the value of $K_F$, $K_G$ and $K_H$ with respect to $\tilde{k}_{\text{max}} \Delta x$. For the same $\Delta x$, the curve of $K_G$ is identical to $K_F$ in Figure 4.4. In Figure 4.5, $K_H$ is always greater than $K_F$ with the same filtering wavenumber $\tilde{k}_{\text{max}}$ when $\Delta x = 2$ mm, $K_H$ is smaller than $K_F$ in the range of $\frac{7\pi}{10} < \tilde{k}_{\text{max}} \Delta x < \frac{4\pi}{5}$ when $\Delta x = 1$ mm and $K_H$ is smaller than $K_F$ in the range of $\frac{3\pi}{5} < \tilde{k}_{\text{max}} \Delta x < \frac{9\pi}{10}$ when $\Delta x = 0.5$ mm.

### 4.4 Spatial Filtering

#### 4.4.1 Discrete Sine and Cosine Transform

The filtered FDTD method extends the CFL limit conditionally by filtering out the high frequency components in the spatial domain. To obtain the spatial frequency components, many techniques, such as the discrete Fourier transform (DFT) and the discrete sine/cosine transform (DST/DCT), can be applied to transform the electromagnetic field from the spatial domain to the spatial frequency domain [78][79]. The DFT is widely used for spectral analysis due to the accurate representation of a signal in the frequency domain. This thesis selects the DST/DCT for implementing the filtered FDTD method. There are two advantages of the DST/DCT over the DFT. The first one is that the computational complexity of the DST/DCT is simpler than the DFT. The DST/DCT computes...
only the real part of the input signals while DFT computes both the real and imaginary part. The second one is that the DST/DCT is odd/even symmetric at the boundaries of the input signals. The DFT repeats the input signal periodically, which may create spurious high frequencies from the boundary discontinuity. However, assuming the input signal to be odd/even symmetric, the boundaries of the DST/DCT computation tend to be continuous. For example, if the input signal is an array of ‘ABCDE’, the DCT computation treats it as a periodical array of ‘ABCDEEDCBA’ and the DST computation treats it as ‘ABCDE0(-E)(-D)(-C)(-B)(-A)’. In the spatial filtering approach, both DST or DCT can be applied to transform the electromagnetic fields from the spatial domain into the spatial frequency domain without creating spurious high frequencies from the boundary discontinuity. DCT is adopted in this thesis for implementing the spatial filtering procedure.

4.4.2 Low Pass Filter in the Spatial Frequency Domain

Instead of modifying the conventional Yee’s equations, the filtered FDTD method introduces a low pass filter to remove the unstable spatial frequency components. In the spatial frequency domain, the two dimensional low-pass filter is defined as

\[ F(\hat{k}_x, \hat{k}_y) = \begin{cases} 1, & \sqrt{\hat{k}_x^2 + \hat{k}_y^2} \leq \hat{k}_{\text{max}} \\ 0, & \sqrt{\hat{k}_x^2 + \hat{k}_y^2} > \hat{k}_{\text{max}} \end{cases} \] (4.19)

Note that, the ideal low pass filters of (4.19) is the only filter that can be applied in the filtered FDTD method. The numerical dispersion rises in the coming time steps, if the unstable spatial components are not removed completely. Thus, other filters, like the Butterworth filter or Chebyshev filter, may cause late time instability.

4.4.3 Procedures

To maintain the stable computation with \( \Delta t \) greater than the CFL limit, the spatial filtering procedure should be applied at each time steps. Figure 4.8 shows the flowchart of the conventional FDTD method and the filtered FDTD method. Figure 4.9 shows the flowchart for the filtered FD-FDTD method with CFS-PML. Since the filtering approach does not reformulate the conventional Yee equations,
Figure 4.6: Transformation from the spatial domain to the spatial frequency domain. The FDTD space has $N_x \times N_y$ cells.

Figure 4.7: Transformation from the spatial frequency domain to the spatial domain. The FDTD space has $N_x \times N_y$ cells.
the filtered FDTD method remains second order accuracy for the numerical approximation.

As shown in Figure 4.9, at $t = (n + \frac{1}{2})\Delta t$, $H_x$, $H_y$ and $H_z$ are updated by the Yee algorithm with the filtered electromagnetic fields. The outgoing waves in the magnetic field are absorbed by the CFS-PML. However, since $\Delta t$ is greater than the CFL limit, unstable harmonics are generated in the magnetic field, especially in the high spatial frequencies. As shown in Figure 4.6, the magnetic field is transformed to spatial frequency domain by using DCT. With the low pass filter in (4.19), Figure 4.7 filters out the wavenumbers that are higher than $\tilde{k}_{max}$ and applies the inverse DCT to obtain the filtered magnetic field. Then, at $t = (n + 1)\Delta t$, the electric field is updated by the Yee algorithm with the filtered magnetic field at $t = (n + \frac{1}{2})\Delta t$. Theoretically, we should apply the filtering procedure to the electric field as well. However this procedure can be excluded by reducing the value of $\tilde{k}_{max}$ or using the $\Delta t$ which is smaller than the upper limit of the revised CFL condition [14].
The Conventional FDTD Method

Start
$t = 0$

$t = t + \frac{1}{2} \Delta t$

Update the magnetic field components $H_x$, $H_y$ and $H_z$ by Yee algorithm

$t = t + \frac{1}{2} \Delta t$

Source excitation $E_z = \text{source (hard source)}$ or $E_z = E_z + \text{source (soft source)}$

Update the electric field components $E_x$, $E_y$ and $E_z$ by Yee algorithm

$t \leq t_{\text{max}}$

Yes

No

End simulation

The Filtered FDTD Method

Start
$t = 0$

$t = t + \frac{1}{2} \Delta t$

Update the magnetic field components $H_x$, $H_y$ and $H_z$ by Yee algorithm

Apply the CFS-PML into the magnetic fields

Transform the magnetic field components to the spatial frequency form of $H_{kx}$, $H_{ky}$ and $H_{kz}$ by DCT

Obtain the filtered magnetic field components $H_{k_{\text{max}}x}$, $H_{k_{\text{max}}y}$ and $H_{k_{\text{max}}z}$ by filtering out the high spatial frequency components

Transform the filtered magnetic field components to the spatial domain form of $H_{x_{\text{filtered}}}$, $H_{y_{\text{filtered}}}$ and $H_{z_{\text{filtered}}}$ by IDCT

$t = t + \frac{1}{2} \Delta t$

Source excitation $E_z = \text{source (hard source)}$ or $E_z = E_z + \text{source (soft source)}$

Update the electric field components $E_x$, $E_y$ and $E_z$ with $H_{x_{\text{filtered}}}$, $H_{y_{\text{filtered}}}$ and $H_{z_{\text{filtered}}}$ by Yee algorithm

Apply the CFS-PML into the electric fields

Repeat the spatial filtering procedure for the electric field components to obtain $E_{x_{\text{filtered}}}$, $E_{y_{\text{filtered}}}$ and $E_{z_{\text{filtered}}}$

$t \leq t_{\text{max}}$

Yes

No

End simulation

Figure 4.8: Flowchart of the conventional FDTD method and the filtered FDTD method.
The Filtered FD-FDTD Method with CFS-PML

Start

\[ t = 0 \]

\[ t = t + \frac{1}{2} \Delta t \]

Update the magnetic field components \( H_x, H_y \) and \( H_z \) by Yee algorithm

Apply the CFS-PML into the magnetic fields

Transform the magnetic field components to the spatial frequency form of \( H_{k_x}, H_{k_y} \) and \( H_{k_z} \) by DCT

Obtain the filtered magnetic field components \( H_{k_{max}}^{x}, H_{k_{max}}^{y} \) and \( H_{k_{max}}^{z} \) by filtering out the high spatial frequency components

Transform the filtered magnetic field components to the spatial domain form of \( H_{filtered}^{x}, H_{filtered}^{y} \) and \( H_{filtered}^{z} \) by IDCT

Source excitation
\( D_z = \text{source (hard source)} \) or
\( D_z = D_z + \text{source (soft source)} \)

Update the electric flux density field components \( D_x, D_y \) and \( D_z \) with \( H_{filtered}^{x}, H_{filtered}^{y} \) and \( H_{filtered}^{z} \)

Update the electric field components \( E_x, E_y \) and \( E_z \) by ADE scheme

Apply the CFS-PML into the electric fields

Repeat the spatial filtering procedure for the electric field components to obtain \( E_{x_{filtered}}, E_{y_{filtered}} \) and \( E_{z_{filtered}} \)

Yes

No

End simulation

\[ t \leq t_{max} \]

\[ t = t + \frac{1}{2} \Delta t \]

\[ t = t + 1 \]

Figure 4.9: Flowchart of the Filtered FD-FDTD method with CFS-PML.
Chapter 5

Numerical Experiments of the Spatial Filtering Approach

The FDTD method becomes a widely used tool for solving the electromagnetic problems in modern engineering. Programmers can easily write the FDTD’s explicit equations using such computer languages as C, C++, JAVA, MATLAB and FORTRAN. As a scientific programming language, FORTRAN is more efficient than many other languages for its concise array operations. Therefore all the numerical tests in this thesis are simulated by FORTRAN in the Linux workstation.

By filtering out the spurious frequency components in the electromagnetic field, the spatial filtering procedure extends the CFL limit conditionally. The key point of realizing the spatial filtering approach is to select the electromagnetic field for filtering. This chapter presents the way to select fields for filtering based on the numerical experiments in the filtered FDTD method and the filtered FD-FDTD method with CFS-PML ABC.

5.1 Experiments of the Filtered FDTD Method

Table 5.1 shows the basic parameters for the filtered FDTD method with lossless materials. Under this condition, the electromagnetic field is excited by the Gaussian derivative pulse of

\[
E_{source}(t) = -100 \frac{t - t_0}{\sqrt{2\pi \tau}} e^{-\frac{(t - t_0)^2}{2\tau^2}}
\]  

(5.1)
Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed of light $c$ (m/s)</td>
<td>$3 \times 10^8$</td>
</tr>
<tr>
<td>Vacuum magnetic permeability $\mu_0$ (H/m)</td>
<td>$4\pi \times 10^{-7}$</td>
</tr>
<tr>
<td>Relative magnetic permeability $\mu_r$ (H/m)</td>
<td>1</td>
</tr>
<tr>
<td>Magnetic permeability $\mu = \mu_0 \cdot \mu_r$ (H/m)</td>
<td>$4\pi \times 10^{-7}$</td>
</tr>
<tr>
<td>Vacuum electrical permittivity $\varepsilon_0 = \frac{1}{c^2 \mu}$ (F/m)</td>
<td>$\frac{1}{36\pi} \times 10^{-9}$</td>
</tr>
<tr>
<td>Relative electrical permittivity $\varepsilon_r$ (F/m)</td>
<td>1</td>
</tr>
<tr>
<td>Electrical permittivity $\varepsilon = \varepsilon_0 \cdot \varepsilon_r$ (F/m)</td>
<td>$\frac{1}{36\pi} \times 10^{-9}$</td>
</tr>
<tr>
<td>Source type</td>
<td>soft</td>
</tr>
</tbody>
</table>

Table 5.1: The simulation parameters for the filtered FDTD method.

where $t_0 = 0.33$ ns and $\tau = 60$ ps [80][81]. Figure 5.1 shows the source excitation in time and Figure 5.2 shows the spectrum of the excitation. According to the definition in [82], the lowest frequency of interest is 0.62 GHz and the highest frequency of interest is $f_{\text{highest}} = 5.73$ GHz. This section shows the numerical results of the filtered FDTD method.

### 5.1.1 2D Filtered FDTD Method

The two dimensional filtered FDTD method is implemented in the TM mode, which consists of $H_x$, $H_y$ and $E_z$. The computation space is discretized by 200 $\times$ 200 Yee cells and each cell is a 1 mm $\times$ 1 mm square. The temporal interval of the filtered FDTD method is defined as $\Delta t = CFLN \times \Delta t_{cfl}$, where CFLN is the CFL number and $\Delta t_{cfl}$ is the maximum temporal interval under the CFL condition. Since $\Delta x = \Delta y = 1$ mm, the maximum wavenumber that our simulation can accommodate is $\tilde{k}_0 = 1000\pi$ rad/m and $\Delta t_{cfl}$ is 2.36 ps. Figure 5.3 shows the simulation setting where the source is excited at $(100,100)$ in the $E_z$ field and the observation point is at $(90,100)$.

Based on the filtering procedures shown in Section 4.4.3, we filter out the spatial frequency components whose wavenumbers are higher than 2200$\pi$ rad/m in both the electric field and magnetic field. With the revised CFL condition (4.6), for $\tilde{k}_{\text{max}} = 220\pi$ rad/m and $\Delta x = 1$ mm, the upper limit of $\Delta t$ is $4.13\Delta t_{cfl}$. 

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Figure 5.1: The source excitation in the time domain.

Figure 5.2: The normalized spectrum of the source excitation. The maximum frequency of this source is $f_{\text{highest}} = 5.73 \text{ GHz}$ and the minimum frequency of this source is $0.62 \text{ GHz}$. 
Figure 5.3: The simulation environment. The computation domain is a 2D cavity filled with air and bounded by PEC. The source is excited in the centre of the $E_z$ field. The observation point is 10 cells away from the excitation point.

Figure 5.4: The electric field distribution of $E_z$ before filtering at $t = 80\Delta t_{cfl}$. 

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Figure 5.5: The spatial spectrum of the electric field distribution of $E_z$ before filtering at $t = 80\Delta t_{cfl}$.

Figure 5.6: The spatial spectrum of the electric field distribution of $E_z$ after filtering at $t = 80\Delta t_{cfl}$. The filtering wavenumber $\tilde{k}_{max}$ is $220\pi$ rad/m.
Hence we set CFLN to 4 in this test.

Figure 5.4 shows the electric field distribution of $E_z$ before filtering at $t = 80\Delta t_{cfl}$. As $\Delta t$ is four times greater than the CFL limit, the unstable components are generated in the computational domain. These components may grow up and cause late time instability.

Figure 5.5 shows the spatial spectrum of $E_z$. Many spurious frequency components are generated in the high spatial frequencies. Figure 5.6 displays the spatial spectrum after filtering out the spatial frequency components whose wavenumbers are higher than $220\pi$ rad/m. Figure 5.7 displays the filtered $E_z$ field in the spatial domain. By using the spatial filtering procedure, the unstable components in Figure 5.7 is less than those in Figure 5.4.

5.1.2 Observed Signals

By filtering out the high spatial frequency components whose wavenumbers are higher than $220\pi$ rad/m in both the electric field and magnetic field, the computation is stable within $10^8$ time steps with CFLN=4. However, as suggested in Section 4.4.3, the filtering procedure can be applied only in the electric field or magnetic field. To determine the field for filtering, we compare the observed signals in the filtered FDTD method and the conventional FDTD method. Figure
Figure 5.8: The observed signals at (90,100) in $E_z$ for four scenarios. The four scenarios are introduced in Table 5.2. In Scenarios 2, 3 and 4, $\hat{k}_{max} = 220\pi$ rad/m and CFLN=4.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>The conventional FDTD method with CFLN=1.</td>
</tr>
<tr>
<td>2</td>
<td>The filtered FDTD method that applies the low pass filter in both $E$ and $H$. DCT technique is used and source is excited in $E$ field.</td>
</tr>
<tr>
<td>3</td>
<td>The filtered FDTD method that applies the low pass filter only in $E$. DCT technique is used and source is excited in $E$ field.</td>
</tr>
<tr>
<td>4</td>
<td>The filtered FDTD method that applies the low pass filter only in $H$. DCT technique is used and source is excited in $E$ field.</td>
</tr>
</tbody>
</table>

Table 5.2: The four scenarios in the numerical experiments.
Figure 5.9: The maximum CFLN which gives stable computation with for each $k_{\text{max}}$. The theoretical value is obtained from (4.6).

5.8 shows the signals observed at $(90,100)$ in $E_z$ for four scenarios which are introduced in Table 5.2. All these scenarios excite the source at electric field. Scenario 1 updates the electromagnetic fields by using the conventional FDTD method. Transforming the electromagnetic fields between spatial and spatial frequency domain via DCT/IDCT technique, the spatial filtering procedure is applied in Scenarios 2, 3 and 4 to gain larger time step, which is set to CFLN=4. As a reference, the observed signal in scenario 1 is obtained from the conventional FDTD method with CFLN=1. The signals observed in are obtained from the filtered FDTD method with different filtered fields. As shown in Figure 5.8, the variation among the observed signals in scenario 1, 2 and 3 is negligible, however the observed signal in scenario 4 is different from the reference in scenario 1. Thus, in the TM mode, to guarantee the accuracy, the electric field should be filtered. Furthermore, in our 2D test for the TE mode with the excitation in either the electric field or magnetic field, the magnetic field has to be filtered because only filtering the unstable components in the electric field causes incorrect results.

5.1.3 Improvement of Computational Efficiency

As discussed in Section 5.1.2 for the TM mode, the filtered FDTD method can be implemented by removing the spurious frequency components in both the electric and magnetic fields or only the electric field. The results of the stability test for
the TM mode are plotted in Figure 5.9. The $y$-axis of Figure 5.9 represents the maximum CFLN that gives stable computation at each $\tilde{k}_{\text{max}}$. The results of the numerical experiments are stable with the maximum CFLN obtained from (4.6). At each $\tilde{k}_{\text{max}}$, the maximum CFLN that gives stable computation with two filtered fields (both $E$ and $H$) is slightly greater than one filtered field (only $E$).

The improvement of the computational efficiency is defined as

$$W = \frac{\text{The run time of the conventional FDTD}}{\text{The run time of the filtered FDTD}}$$

where the run time of the conventional FDTD is measured with CFLN=1 for 10000 time steps and the run time of the filtered FDTD is measured for $\frac{10000}{\text{CFLN}}$ time steps. Figure 5.10 shows that, in the 2D filtered FDTD method, the computational speed of applying the filtering procedure in two fields is faster than the conventional FDTD method when CFLN is greater than 9. However, for the filtered FDTD method with one filtered field, the computational speed is faster than the conventional FDTD method when CFLN is greater than 3. Thus, although implementing the filtering procedure to both $E$ and $H$ fields slightly increases the maximum CFLN for stable computation, its computational speed is about three times slower than that of the case for applying the low-pass filter to only the electric field.
5.2 Experiments of the Filtered FD-FDTD Method with CFS-PML

5.2.1 Relative Permittivity of Debye Media

This section presents the numerical experiments of the filtered FD-FDTD method with CFS-PML. Based on the definition in (2.57), the relative permittivity in the one-pole Debye model is expressed as

\[ \varepsilon_r = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau_D} + \frac{\sigma}{j\omega\varepsilon_0}. \]  

(5.3)

Thus the revised CFL condition of the filtered FDTD method is obtained by replacing \( c \) with

\[ v = \frac{1}{\sqrt{\varepsilon\mu}} = \frac{c}{\sqrt{\varepsilon_r\mu_r}} \]  

(5.4)

where \( v \) is the speed of wave propagation in the dispersive medium, for equations (4.3), (4.6) and (A.3).

5.2.2 Scaling of the PML Conductivity

If the PML conductivity \( \sigma_x \) in (2.82) is regarded as a lossy constant, a spurious reflection is produced at the PML interface [35]. To improve this phenomenon, the PML conductivity \( \sigma_x \) has to be growing from an infinitesimal value at the interior-PML interface to the relatively high value at the bound of PML layers. Practically, scaled by a geometrical progression, the PML conductivity \( \sigma_x \) in the \( x \)-direction is defined as

\[ \sigma_x(d) = \sigma_0 \left(g^{1/\Delta x}\right)^d \]  

(5.5)

where \( g \) is the scaling factor that determines the increment from one FDTD cell to the next, \( d \) is the distance from the interior-PML interface and \( \sigma_0 \) is the initial value for \( \sigma_x \) at the interface [35]. \( \sigma_0 \) is given as

\[ \sigma_0 = -\frac{\varepsilon_0 c \ln g \ln (R_0)}{2\Delta x (g^N - 1)} \]  

(5.6)
Figure 5.11: The simulation environment. The computational domain is a 2D cavity filled with Debye media. 32 CFS-PML layers are applied into this computational domain. The excitation point is 10 cells away from the centre of the whole domain, and the observation point is 10 cells away from the excitation point.

where $N$ is the number of total PML layers, $R_0$ is the reflection coefficient [35]. In this thesis, the scaled PML conductivity is produced by $g = 1.2$, $N = 32$ and $R_0 = 10^{-4}$.

### 5.2.3 2D Filtered FD-FDTD Method with CFS-PML

Figure 5.11 shows the simulation environment of the 2D filtered FD-FDTD method with CFS-PML in the TM mode. The FDTD space of 200 × 200 cells is truncated by the PEC boundary. Each cell is a 1 mm × 1 mm square. 32 CFS-PML layers are applied to absorb the outgoing waves. The whole computational domain is filled with fat and excited at (90,100) with the source in (5.1). To extend the CFL limit, the spatial filter can be carried out either before or after applying the boundary conditions. However, in the numerical tests, the accuracy of implementing the filtering procedure after applying the boundary conditions is better than before applying the boundary conditions.
5.2.4 Observed Signals

The one-pole Debye model is implemented by the ADE scheme, which consists of $H$, $D$ and $E$. In our tests, the filtered FD-FDTD method cannot extend the CFL limit by applying the filtering procedure only in the $D$ field. Figure 5.12 shows the signal observed at (80,100) for four scenarios. The input signal of these four scenarios are excited in the electric field. Scenario 1 is the case of conventional FD-FDTD method with CFS-PML. Scenarios 2, 3 and 4 are the cases of filtered FD-FDTD method with CFS-PML by using DCT/IDCT technique to transform the field components between spatial domain and spatial frequency domain. Scenario 2 applies the filtering procedure in both $E$ and $H$ fields, Scenario 3 applies the filtering procedure only in $E$ field and Scenario 4 applies the filtering procedure only in $H$ field. The observation in scenario 1 is obtained by setting CFLN=1. CFLN is set to 4 in Scenarios 2, 3 and 4. For the filtered FD-FDTD method, except for the scenario 4, the results of the rest scenarios are identical to reference in scenario 1. Thus, in the TM mode, the filtering procedure can be applied in only $E$ or both $E$ and $H$. In the further numerical experiments for the TE mode, the magnetic field should be filtered because only filtering the electric field gives the incorrect results.
Figure 5.13: The maximum CFLN which gives stable computation for each \( \tilde{k}_{\text{max}} \).

The theoretical value is obtained from (4.6).

Figure 5.14: The improvement of computational efficiency.
5.2.5 Improvement of Computational Efficiency

Figure 5.13 compares the maximum CFLN that gives stable computation in the numerical experiments with the theoretical value in (4.6). The maximum CFLN for the filtered FDTD method with two filtered fields (\(E\) and \(H\)) is greater than the theoretical value when \(\tilde{k}_{\text{max}}\) is smaller than 200\(\pi\) rad/m. For the case with one filtered field (only \(E\)), the maximum CFLN of the numerical experiments is greater than the theoretical value when \(\tilde{k}_{\text{max}}\) is smaller than 120\(\pi\) rad/m. From \(\tilde{k}_{\text{max}} = 330\pi\) rad/m to 1000\(\pi\) rad/m, the maximum stable CFLN of these two kinds of filtering implementations are the same as the theoretical value. Figure 5.14 shows the improvement of the computational efficiency in the filtered FDTD method. With the same CFLN, the computational efficiency for filtering both \(H\) and \(E\) decreases about three times in comparison to the scenario that only applies the spatial filtering procedure to \(E\). Since the maximum stable CFLN in the numerical experiments with one filtered field is similar to that with two filtered field, we can filter only the electric field in the 2D TM mode.
Chapter 6

Analysis of the Numerical Results

For the spatial filtering approach, the upper limit of $\Delta t$ is obtained by the revised CFL condition with a given $\tilde{k}_{\text{max}}$. In [13][14], the lower bound of $\tilde{k}_{\text{max}}$ is defined as $\frac{\pi}{\Delta x}$ to minimize the numerical dispersion. However, the numerical dispersion of the filtered FDTD method depends on both $\Delta x$ and the frequency of excitation. In addition, other aspects such as the spectrum of the excitation and the absorbing ability of the PML are affected by the filtering procedure when $\tilde{k}_{\text{max}}$ is small. To find the optimized $\tilde{k}_{\text{max}}$, the chapter investigates major factors that affect the stability and accuracy of the filtered FD-FDTD method with CFS-PML ABC.

6.1 Simulation Settings

In the 2D TM mode, removing the high spatial frequency components only in the electric field, the filtered FD-FDTD with CFS-PML method was tested with the FDTD sizes of $200 \times 200$ cells, $400 \times 400$ cells and $1600 \times 1600$ cells. The spatial size of the Yee cells is $\Delta x = \Delta y = 1$ mm. Thus $\tilde{k}_0 = 1000\pi$ rad/m and $\Delta t_{\text{cfl2d}} = 2.36$ ps. As the same simulation environment in Figure 5.11, the FDTD space is terminated with the CFS-PML and excited ten cells away from the centre with the source in (5.1). The entire computational domain is filled with either air or fat. Based on these two cases, the performance of the spatial filtering approach with dispersive material is analyzed.
Figure 6.1: The maximum CFLN which gives stable computation for each $\tilde{k}_{max}$ with different PML layers in air. Theoretical values are obtained from (4.6). The shadow area is enlarged to display more details. The FDTD space is $200 \times 200$ cells.

### 6.2 Analysis for the Stability

Both the dispersive material and the conductivity of CFS-PML influence the upper limit of $\Delta t$ for stable computations in the spatial filtering approach. In the conventional FDTD method, with the same $\Delta x$, the maximum $\Delta t$ for stable computation is identical for any sizes of the FDTD space. However, in the filtered FDTD method, the upper limit of $\Delta t$ is impacted by the FDTD sizes with the same $\Delta x$. Thus this section analyzes the stability of the filtered FD-FDTD method with CFS-PML based on the sizes of the FDTD space.

#### 6.2.1 PML Conductivity

As shown in (5.5) and (5.6), the scaled $\sigma_x(d)$ is obtained by three variables of $g$, $R_0$ and $N$. With $g = 1.2$ and $R_0 = 10^{-4}$, Figure 6.1 displays the maximum CFLN that gives stable computation for $N = 4, 8$ and $32$ in the FDTD space of $200 \times 200$ cells. The maximum stable CFLN of the numerical experiments are equal to or greater than the theoretical values which are obtained from (4.6).
upper limit of the CFLN is decreased slightly by reducing the layers of the CFS-PML. In the further tests for the reflection coefficient $R_0$ and the scaling factor $g$, the maximum stable CFLN decreases by increasing $g$ and $R_0$. In the numerical experiments with the FDTD space of $400 \times 400$ cells and $1600 \times 1600$ cells, the influence of $g$, $R_0$ and $N$ on the stability are the same as those of $200 \times 200$ cells.

6.2.2 Comparison between Air and Fat media

6.2.2.1 In Air

Figure 6.2 shows the results of the stability test with 32 CFS-PML layers in air. The upper limit of the CFLN for stable computation decreases when the size of the FDTD space increases. In the range of $\tilde{k}_{max} < 500\pi$ rad/m, the stability performance for the FDTD space of $200 \times 200$ cells is better than the cases of $400 \times 400$ and $1600 \times 1600$ cells, and the case of $400 \times 400$ cells is better than $1600 \times 1600$ cells. The maximum stable CFLN in the FDTD space of $1600 \times 1600$ cells almost coincides with the theoretical curve.
6.2.2.2 In fat

Figure 6.3 displays the results of the stability test with 32 CFS-PML layers in fat. At the highest excited frequency of 5.73 GHz, the relative permittivity of fat increases 5.53 times in comparison to the air. Due to the increment of the relative permittivity, based on (4.6) and (5.4), the theoretical value for the maximum stable CFLN in fat is 2.35 times greater than that in air. As shown in Figure 6.3, the maximum stable CFLN in the numerical experiments is smaller than the theoretical value when $\tilde{k}_{max}$ is large. In the case of 400 × 400 cells, the maximum stable CFLN is greater than the theoretical value when $\tilde{k}_{max}$ is less than $100\pi$ rad/m. However the maximum stable CFLN in the FDTD space of 1600 × 1600 cells is always smaller than the theoretical value by one or two. Thus, with the dispersive materials, the capability of the spatial filtering approach to extend the CFL limit is decreased.

6.2.3 Improvement of the Computational Efficiency

Figure 6.4 shows the improvement of the computational efficiency $W$ for three FDTD sizes. In the two dimensional computation, the filtered FD-FDTD method
costs less execution time than the conventional FD-FDTD method when CFLN is equal to or greater than two.

6.3 Analysis for the Accuracy

6.3.1 Numerical Phase Velocity of the Filtering Approach

As mentioned in Section 3.4, the variation between the numerical propagation velocity and the physical propagation velocity is the key point to evaluate the numerical dispersion. Substituting the upper limit of $\Delta t$ in (4.6) into (3.38), for the wave propagating along the major grid axes ($\varphi = 0, \pi/2, \pi$ and $3\pi/2$), the numerical phase velocity of the spatial filtering approach is expressed as

$$\tilde{c}_{2D_{filter1}} = \frac{\omega \Delta x}{2 \arcsin \left( \sqrt{2} \sin \left( \frac{k_{max} \Delta x}{2\sqrt{2}} \right) \sin \left( \frac{\omega \Delta x}{c2\sqrt{2} \sin \left( \frac{k_{max} \Delta x}{2\sqrt{2}} \right)} \right) \right)}.$$

Figure 6.4: The improvement of computational efficiency for three FDTD sizes.
Figure 6.5: The numerical phase velocity errors for $\Delta x = \frac{\lambda_{\text{min}}}{10}$, $\frac{\lambda_{\text{min}}}{20}$, $\frac{\lambda_{\text{min}}}{40}$ and $\frac{\lambda_{\text{min}}}{32.4}$. $\lambda_{\text{min}}$ is 5.24 cm. $\Delta x = \frac{\lambda_{\text{min}}}{32.4}$ is the spatial size used in the numerical experiments. $P_{2D}$ is obtained from (3.41).

Substituting the upper limit of $\Delta t$ in (4.6) into (3.40) yields

$$\tilde{c}_{2D_{\text{filter}}} = \frac{\omega \Delta x}{2\sqrt{2} \arcsin \left( \frac{\sin \left( \frac{\tilde{k}_{\text{max}} \Delta x}{2\sqrt{2}} \right) \sin \left( \frac{\omega \Delta x}{c2\sqrt{2}\sin \left( \frac{\tilde{k}_{\text{max}} \Delta x}{2\sqrt{2}} \right)} \right)} \right)}$$

which is the numerical phase velocity of the propagation angles of $\varphi = \pi/4$, $3\pi/4$, $5\pi/4$ and $7\pi/4$ in the spatial filtering approach.

Figure 6.5 shows the numerical phase velocity error of the spatial filtering approach. At each value of $\tilde{k}_{\text{max}} \Delta x$, the numerical phase velocity error $P_{2D}$ reduces when $\Delta x$ decreases. Figure 6.6 shows the anisotropy error of the spatial filtering approach. The numerical velocity anisotropy error $P_{2D_a}$ reduces with decreasing $\Delta x$.

The highest excited frequency of the source in (5.1) is 5.73 GHz, thus the minimum wavelength of the excitation is 5.24 cm. In the numerical experiments, $\Delta x$ is 1 mm, which equals $\frac{\lambda_{\text{min}}}{32.4}$. As shown in Figure 6.5, for the case of $\Delta x = \frac{\lambda_{\text{min}}}{32.4}$, when $\tilde{k}_{\text{max}}$ is smaller than $20\pi$ rad/m, $P_{2D}$ is greater than one. At $\tilde{k}_{\text{max}} = 1000\pi$
rad/m, the numerical phase velocity error of the filtered FDTD method is identical to the numerical phase velocity error of the conventional FDTD method. The numerical velocity anisotropy error of our tests is shown in Figure 6.6 with \( \Delta x = \frac{\lambda_{\text{min}}}{10} \), \( \frac{\lambda_{\text{min}}}{20} \), \( \frac{\lambda_{\text{min}}}{40} \) and \( \frac{\lambda_{\text{min}}}{52.4} \). \( \lambda_{\text{min}} \) is 5.24 cm. \( \Delta x = \frac{\lambda_{\text{min}}}{52.4} \) is the spatial size used in the numerical experiments. \( P_2D_a \) is obtained from (3.42).

6.3.2 Spectrum Loss of the Excitation signal due to the Filtering Procedure

As reported in [51], the numerical dispersion reduces while \( \Delta t \) approaches to the CFL limit. Thus \( \Delta t \) is set to \( \frac{\Delta x}{\sqrt{2}c} \) for the 2D FDTD computation in the case of \( \Delta x = \Delta y \). The maximum frequency that the numerical computation can afford is \( \tilde{f}_0 = \frac{1}{2\Delta t} = \frac{c}{\sqrt{2}\Delta x} = \frac{c_{\tilde{k}_0}}{\sqrt{2}\pi} \). In order to relax the CFL condition, the field components in the wavenumbers from \( \tilde{k}_{\text{max}} \) to \( \tilde{k}_0 \) are removed in the filtered FDTD method. Therefore the frequency components from \( \frac{c_{\tilde{k}_{\text{max}}}}{\sqrt{2}\pi} \) to \( \tilde{f}_0 \) are affected by the spatial filtering procedure while the electromagnetic waves are...
propagating through the FDTD space. For the excitation with wide bandwidth, if part of the frequencies of the excitation are greater than \( \frac{c \tilde{k}_{\text{max}}}{\sqrt{2}\pi} \), the accuracy of the calculation is affected by both the dispersion error and spectrum loss. The spectrum loss \( \mathcal{E} \) of the excitation signal is expressed as

\[
\mathcal{E} = \sqrt{\frac{\sum_{l=1}^{T} |s_{\text{nofilter}}(l) - s_{\text{filtered}}(l)|^2}{\sum_{l=1}^{T} |s_{\text{nofilter}}(l)|^2}} \quad (6.3)
\]

where \( T \) is the number of maximum time steps,

\[
s_{\text{nofilter}}(l) = 2 \frac{T}{T/2} \sum_{m=1}^{T/2} S(m) \exp \left( \frac{j2\pi lm}{T} \right), \quad (6.4)
\]

\[
s_{\text{filtered}}(l) = 2 \frac{T}{T} \sum_{m=1}^{T} S(m) \exp \left( \frac{j2\pi lm}{T} \right). \quad (6.5)
\]

In (6.4) and (6.5), \( S(m) \) is the spectrum of the excitation and \( T_f = \tilde{f}_{\text{max}} / \Delta f \), where \( \Delta f = 1/(T\Delta t) \) and \( \tilde{f}_{\text{max}} = c\tilde{k}_{\text{max}}/(\sqrt{2}\pi) \). Note that, (6.3) is the deviation between the filtered signal and the non-filtered signal in time domain. \( s_{\text{nofilter}}(l) \) and \( s_{\text{filtered}}(l) \) are derived from \( S(m) \) by using the inverse discrete Fourier transform. Substitution of (6.4) and (6.5) into (6.3) yields

\[
\mathcal{E} = \sqrt{\frac{\sum_{l=1}^{T} \left| \sum_{m=T_{f}+1}^{T/2} S(m) \exp \left( \frac{j2\pi lm}{T} \right) \right|^2}{\sum_{l=1}^{T} \left| \sum_{m=1}^{T} S(m) \exp \left( \frac{j2\pi lm}{T} \right) \right|^2}} \quad (6.6)
\]

The simulation error \( \mathcal{R} \) between the conventional FD-FDTD method and the filtered FD-FDTD method is calculated by

\[
\mathcal{R} = \sqrt{\frac{\sum_{i} |F_{\text{filtered}}(i\Delta t, \tilde{k}_{\text{max}}, CFLN) - F_{\text{nofilter}}(i\Delta t)|^2}{\sum_{i} |F_{\text{nofilter}}(i\Delta t)|^2}} \quad (6.7)
\]
Figure 6.7: The theoretical spectrum loss of the excitation $E$ and the simulation error $R$. The FDTD size is $200 \times 200$ cells and 32 CFS-PML layers were used. The computational domain is filled with air.

where $F_{\text{filtered}}$ and $F_{\text{nofilter}}$ represent the observed signals in time domain for the filtered and conventional FDTD method, respectively.

Figure 6.7 compares the spectrum loss of excitation with the calculated error of simulation results. In Figure 6.7 $\mathcal{R}$ is greater than 100% in the range of $\tilde{k}_{\text{max}} < 20\pi$ rad/m. This is caused by the numerical phase velocity error as shown in Figure 6.5. However, the error of simulation is about 10% higher than $E$ from $\tilde{k}_{\text{max}} = 20\pi$ rad/m to $120\pi$ rad/m. This difference is caused by the PML boundary. Figure 6.8 shows the signal observed at (80,100) in $E_z$. With $\tilde{k}_{\text{max}} = 80\pi$ rad/m, the outgoing wave is not completely absorbed by the PML boundary conditions.

6.3.3 Impact to the PML

The conductivity $\sigma_x(d)$ is increased geometrically from the interior-PML interface to the PEC boundary, which absorbs the incident wave rapidly after the wave traveled into the CFS-PML. The strong attenuation of the traveling wave in the CFS-PML causes high spatial frequency components. If these high spatial frequency components are filtered out, the absorbing ability of the PML boundary condition is degraded. Figure 6.8 shows that the absorbing ability of the PML
boundary condition is reduced by decreasing the value of $\tilde{k}_{max}$. The rapid wave attenuation in the CFS-PML causes high spatial frequency components, which requires a high $\tilde{k}_{max}$ to protect the absorbing ability of the CFS-PML. As $\sigma_x(d)$ controls the absorbing ability of the CFS-PML, a well designed $\sigma_x(d)$ can reduce the impact of the spatial filtering approach to the CFS-PML boundary condition. In our simulations, with the $\sigma_x(d)$ of $g = 1.2$ and $R_0 = 10^{-4}$, the filtered FDTD method yields the best accuracy.

As displayed in Figure 6.7, the absorbing ability of the CFS-PML is affected by the spatial filtering procedure when $\tilde{k}_{max}$ is smaller than $180\pi$ rad/m. To match the value of $R$, $\mathcal{E}$ need to be shifted along the positive direction of the $x$-axis by approximately $75\pi$ rad/m.

### 6.3.4 Accuracy Assessment

The simulation error $\mathcal{R}$ of the numerical experiments are calculated by (6.7). We only present $\mathcal{R}$ which is smaller than 50%. Figures from 6.9 to 6.14 show $\mathcal{R}$ with different $\tilde{k}_{max}$ and CFLN in either air or fat. Although the low pass filter is applied only in the electric field, all simulation results show that we can increase
Figure 6.9: The simulation error $\mathcal{R}$ for the FDTD size of $200 \times 200$ in air. $\mathcal{R}$ is calculated by using (6.7).

Figure 6.10: The simulation error $\mathcal{R}$ for the FDTD size of $400 \times 400$ in air. $\mathcal{R}$ is calculated by using (6.7).

Figure 6.11: The simulation error $\mathcal{R}$ for the FDTD size of $1600 \times 1600$ in air. $\mathcal{R}$ is calculated by using (6.7).
Figure 6.12: The simulation error $\mathcal{R}$ for the FDTD size of $200 \times 200$ in fat. $\mathcal{R}$ is calculated by using (6.7).

Figure 6.13: The simulation error $\mathcal{R}$ for the FDTD size of $400 \times 400$ in fat. $\mathcal{R}$ is calculated by using (6.7).

Figure 6.14: The simulation error $\mathcal{R}$ for the FDTD size of $1600 \times 1600$ in fat. $\mathcal{R}$ is calculated by using (6.7).
the CFLN up to 13 with \( R \) smaller than 10%. Obviously, at the same filtering wavenumber \( \tilde{k}_{\text{max}} \), \( R \) increases when CFLN increases.

Comparing to the simulation errors in air, with the same FDTD size, we need a larger \( \tilde{k}_{\text{max}} \) to gain the same \( R \) for the case of fat. For example, in the FDTD space of 200 \times 200 cells with air, \( R \) is smaller than 10% when \( \tilde{k}_{\text{max}} \) is less than 85\( \pi \) rad/m. However, when the computational domain is filled with fat, \( R \) is smaller than 10% when \( \tilde{k}_{\text{max}} \) is less than 125\( \pi \) rad/m.

In the filtering approach, \( R \) decreases by increasing the size of the FDTD space. For the experiments with air, to keep the error less than 10%, the maximum stable CFLN we can use is 10 at \( \tilde{k}_{\text{max}} = 100\pi \) rad/m for the case of 200 \times 200 cells, the maximum stable CFLN is 11 at \( \tilde{k}_{\text{max}} = 90\pi \) rad/m for the case of 400 \times 400 cells and the maximum stable CFLN is 13 at \( \tilde{k}_{\text{max}} = 80\pi \) rad/m for the case of 1600 \times 1600 cells. The accuracy is clearly improved by enlarging the FDTD size for the case of air. However, in the computational domain filled with fat, the accuracy improvement by enlarging the FDTD size is negligible. For example, to keep the error smaller than 10%, the highest CFLN for the all three FDTD sizes are 14 at \( \tilde{k}_{\text{max}} = 150\pi \) rad/m.

6.4 Guidance of Choosing the Filtering Wavenumber

Based on the analysis in Section 6.2 and Section 6.3, we can run simulations as follows:

1. Choose the excitation and the size of the FDTD space.

2. Set the parameters of CFS-PML. These parameters should satisfy condition (3.98).

3. Calculate the numerical velocity error \( P_{2D} \) with respect to \( \tilde{k}_{\text{max}} \) by substituting (6.1) and (6.2) into (3.41).

4. Based on (6.6), calculate the spectrum loss \( E \) with respect to \( \tilde{k}_{\text{max}} \).

5. Add up the results in step 3 and 4 and let \( \mathcal{U}(\tilde{k}_{\text{max}}) = P_{2D}(\tilde{k}_{\text{max}}) + E(\tilde{k}_{\text{max}}) \). \( \mathcal{U}(\tilde{k}_{\text{max}}) \) is the expected simulation error of the filtered FDTD method.

6. Select the \( \tilde{k}_{\text{max}} \) with a desirable accuracy based on \( \mathcal{U}(\tilde{k}_{\text{max}}) \).
7. To reduce the impact of the spatial filtering procedure on PML, an addi-
tional value should be added to the $\hat{k}_{\text{max}}$ which is selected in step 6 (i.e. with the $\sigma_x(d)$ in our test, the additional wavenumber is $75\pi$ rad/m.).

8. Find the CFLN by the revised CFL conditions.

9. Choose the field for filtering based on the results in Chapter 5 and apply the spatial filtering procedure at each time step.

6.5 Practical Application

Following the guidance in Section 6.4, this section shows a realistic test of deep brain stimulation (DBS), which is a biomedical treatment for neurological disorders. The DBS is applicable to treat the symptoms of Parkinson’s disease and essential tremor. The surgical treatment of DBS has some potential risks such as infection, seizure, electrode fracture, skin irritation, intracranial hemorrhage and so on. In order to reduce the risks of surgical treatment, the non-invasive treatment, which stimulates the targeted tissue by exciting the electromagnetic waves outside the human body, is adopted. To simulate non-invasive treatment, the electromagnetic wave propagation in human body is studied by the proposed filtered FD-FDTD method with CFS-PML.

6.5.1 Numerical Modeling of the Human Tissues

The digital human phantom (DHP) used in this project was provided by RIKEN (Saitama, Japan) under no-disclosure agreement between RIKEN and the University of Manchester. The usage was approved by RIKEN ethical committee. To obtain the DHP data for human body, the bio-research infrastructure construction team of RIKEN scanned the human body of a male by using the magnetic resonance imaging (MRI) technique with the spatial resolution of 1 mm. The 3D DHP data is composed of $265 \times 490 \times 1682$ voxels and 53 kinds of tissues \cite{86}. Each voxel is a uniform cell ($1\text{mm}^3$) and can be assembled to represent the human tissues or organs. Table 6.1 shows the parameters for human tissues in the Debye relaxation model \cite{85}. The data is provided by the U.S. Air Force and the parameters are fitted by Fumie’s group \cite{86,87,88}. In 1996, the U.S. Air Force reported their experimental data of the dielectric parameters of human tissues in \cite{87}. Based on their data, the dielectric parameters for Debye model are fitted
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Table 6.1: The parameters for human tissues in the one-pole Debye relaxation model \[83\].
The cross section of the human head on the $xy$-plane at $z = 180$. The simulation environment

Figure 6.15: The cross section of human head on the $xy$-plane at $z = 180$ and the simulation environment. The size of the simulation field is $265 \times 490$ cells and the thickness of the CFS-PML layers is 32 cells. The field is excited at $(130,150)$ and observed at $(130,180)$.

by using Newton’s method and least square fitting method [86]. Each human tissue is assigned with a unique number which is presented in the first column of Table 6.1. For the bio-medical applications, the DHP data can be mapped to the corresponding human body tissues according to this unique number.

6.5.2 Numerical Experiment of Deep Brain Stimulation

The DHP data in this experiment are plotted by a number of portable graymap (PGM) files, which are written in ASCII code. Each PGM file represents one slice of the human body on the $xy$-plane. Thus the size of each PGM file is $265 \times 490$ and the total number of these PGM files is 1682. The left hand side of Figure 6.15 shows the cross section of human head on the $xy$-plane at $z = 180$ and the right hand side of Figure 6.15 shows the simulation environment. The FDTD
The value of $U$, $P_{2D}$ and $\mathcal{E}$ varying $\tilde{k}_{max}$ from zero to 250 $\pi$ rad/m.

With $\Delta x = 1$ mm and the highest excited frequency of 5.73 GHz, the numerical phase velocity error $P_{2D}(\tilde{k}_{max})$ is derived by substituting (6.1) and (6.2) into (3.41). With $T_f = \tilde{f}_{max} / \Delta f = \frac{\tilde{k}_{max}}{\sqrt{2}\pi\Delta f}$ and the spectrum of the excitation, the spectrum loss $\mathcal{E}(\tilde{k}_{max})$ of the excitation is obtained. Then we can derive the expected error of this simulation by using $U(\tilde{k}_{max}) = P_{2D}(\tilde{k}_{max}) + \mathcal{E}(\tilde{k}_{max})$, which is displayed in Figure 6.16. If the expected simulation error is 6.13%, $\tilde{k}_{max}$ is 100$\pi$ rad/m according to the value of $U(\tilde{k}_{max})$. To guarantee the absorbing ability of the CFS-PML, $\tilde{k}_{max} = 175\pi$ rad/m is used in the simulation (at $\tilde{k}_{max} = 175\pi$, $U(\tilde{k}_{max}) = 0.012$). Substituting $\tilde{k}_{max} = 175\pi$ rad/m and $\Delta x = 1$ mm into the revised CFL condition (4.6), the maximum $\Delta t$ for stable computation is $\Delta t = 5.18\Delta t_{cfl2d}$. As shown in Figure 6.3, the stability of the filtered FDTD method can be decreased by the dispersive media. As a results, the CFLN in this application is set to 4. Similarly, if the expected simulation is 0.613%, $\tilde{k}_{max}$ should be set to 300$\pi$ and CFLN=2.

Figure 6.16, Figure 6.18, Figure 6.19, Figure 6.20 and Figure 6.21 compare the electric field distribution in the conventional FDTD method with that in the filtered
FDTD method at \( t = 100\Delta t_{cfl2d} \), \( 200\Delta t_{cfl2d} \), \( 500\Delta t_{cfl2d} \) and \( 1000\Delta t_{cfl2d} \), respectively. The conventional FDTD method is computed with CFLN=1. For the filtered FDTD method, \( \tilde{k}_{max} = 175\pi \text{ rad/m} \) is adopted for the simulation with CFLN=4, \( \tilde{k}_{max} = 300\pi \text{ rad/m} \) is adopted for the simulation with CFLN=2 and \( \tilde{k}_{max} = 1000\pi \text{ rad/m} \) is adopted for the simulation with CFLN=1. Figure 6.17 shows the signals observed at (130,180). The observed signal in the conventional FDTD method with CFLN=1 is used to compare with the signals observed in the filtered FDTD method with CFLN=2 and 4. Based on results in Figure 6.17, the simulation error \( R \) in the filtered FDTD method with CFLN=2 is 5.62% and that with CFLN=4 is 8.15%. At CFLN=4, the simulation error is higher than the expected simulation error (6.13%).
Figure 6.18: Electrical field distribution at $t = 100\Delta t_{\text{eff}}$. 

Conventional FDTD
CFLN=1
Max = 0.0418 V/m
Min = 0 V/m

Filtered FDTD
CFLN=1
Max = 0.0418 V/m
Min = 0 V/m

Filtered FDTD
CFLN=2
Max = 0.0412 V/m
Min = 0 V/m

Filtered FDTD
CFLN=4
Max = 0.0397 V/m
Min = 0 V/m
Figure 6.19: Electrical field distribution at $t = 200\Delta t_{f,2d}$. 

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Figure 6.20: Electrical field distribution at $t = 500\Delta t_{cfl2d}$. 
Figure 6.21: Electrical field distribution at $t = 1000\Delta t_{cfl2d}$. 

Max $(V/m)$

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Chapter 7

Conclusion and Future Work

7.1 Conclusion

The aim of this research project is to improve the computational speed of the FDTD method for biomedical applications. In numerical computing, the biological tissues are regarded as lossy and dispersive materials which are frequency dependent (FD). As a draw back of the FDTD method, the computational efficiency of the FDTD method is constrained by the CFL limit, which defines the upper bound of the temporal size $\Delta t$ for stable computations. To extend the CFL limit, the filtered FDTD method removes the unstable harmonics in the spatial frequency domain by using an ideal low-pass filter. This thesis introduces frequency dependent materials into the filtered FDTD method. The frequency dependent materials are generated by the one-pole Debye model and the outgoing waves are absorbed by the CFS-PML ABC.

Stability and accuracy are crucial for evaluating the performance of the numerical computations. This research implemented the filtered FD-FDTD method with CFS-PML and investigated its stability and accuracy.

Based on the numerical dispersion relation of the CFS-PML, the stability conditions are derived to determine the maximum stable $\Delta t$ for the FDTD method with CFS-PML. The upper limit of $\Delta t$ in the CFS-PML depends on both $\Delta t$ and parameters of the CFS-PML. When the parameters of the CFS-PML are chosen for these stability conditions, the maximum stable $\Delta t$ of the FDTD method with CFS-PML is equal to or greater than the CFL limit.

The filtered FDTD method extends the CFL limit by filtering out the spatial components whose wavenumber is higher than $\tilde{k}_{\text{max}}$. This work introduced the
procedure to realize the filtered FD-FDTD method with CFS-PML and presented the revised stability conditions for the filtered FDTD method with CFS-PML. To implement this method, only filtering the spurious frequency components in the electric field is recommended in the 2D TM mode while only filtering the spurious frequency components in the magnetic field is recommended in the 2D TE mode.

The major aspects that affect the stability and accuracy of the filtered FD-FDTD computation with CFS-PML are investigated. Three major aspects that affect the stability are the conductivity of CFS-PML, the material dispersion and the size of the FDTD space. Three major aspects that affect the accuracy are the numerical dispersion, spectrum loss of the excitation and the reduction of the PML’s absorbing ability. The numerical dispersion is studied based on the numerical phase velocity error. The spectrum loss of the excitation and the reduction of the PML’s absorbing ability are caused by the spatial filtering procedure. Based on the analysis of stability and accuracy, a guidance for choosing \( \tilde{k}_{\text{max}} \) is presented, which provides an expected accuracy for simulation.

The proposed filtered FD-FDTD method with CFS-PML is applied to a practical application for biomedical treatment, where the electromagnetic wave propagation is simulated in human body. The results of the filtered FD-FDTD method with CFS-PML are compared with the conventional FD-FDTD method with CFS-PML.

### 7.2 Future Work

The suggested future works for the filtered FD-FDTD method with CFS-PML are

1. Investigation of the stability condition in 3D. The stability conditions of the filtered FD-FDTD method with CFS-PML is presented in 2D, and can be extended to 3D.

2. Implementation of a faster Fourier transform. The DST/DCT is recommended in this thesis, since DST/DCT only computes the real part of the input signals. The computational speed of the filtered FD-FDTD method with CFS-PML can be further improved by using a faster Fourier transform. The sparse Fourier transform is a suggested scheme [88].

3. Implementation of Huygens subgridding (HSG) scheme. For simulations
with electrically large objects, the subgridding schemes are adopted to improve the computational efficiency. The HSG is a suggested subgridding scheme, since its reflection from the interface of the subdomain is lower than other subgridding schemes [89].

4. Parallelization of the spatial filtering approach to further improve the computational speed.
Appendix A

The 3D filtered FDTD Method

This chapter reviews the revised CFL condition for the 3D filtered FDTD method and introduces spherical excitation to implement the 3D filtered FDTD method.

A.1 Revised 3D CFL Condition

To satisfy any real $\omega$, the 3D numerical dispersion (3.25) can be written as

$$c^2 \Delta t^2 \left( \frac{\sin^2 \left( \frac{k \sin \theta \cos \varphi \Delta x}{2} \right)}{\Delta x^2} + \frac{\sin^2 \left( \frac{k \sin \theta \sin \varphi \Delta y}{2} \right)}{\Delta y^2} + \frac{\sin^2 \left( \frac{k \cos \theta \Delta z}{2} \right)}{\Delta z^2} \right) \leq 1.$$  

(A.1)

If $\Delta x = \Delta y = \Delta z$, filtering out the wavenumbers higher than $\tilde{k}_{\text{max}}$ in (A.1), the revised 3D CFL condition for $\Delta t$ is obtained as

$$\Delta t \leq \frac{\Delta x}{c \sqrt{\sin^2 \left( \frac{k_{\text{max}} \sin \theta \cos \varphi \Delta x}{2} \right) + \sin^2 \left( \frac{k_{\text{max}} \sin \theta \sin \varphi \Delta y}{2} \right) + \sin^2 \left( \frac{k_{\text{max}} \cos \theta \Delta z}{2} \right)}}.$$  

(A.2)

Referring to [14], the minimum value of $K_B(\theta, \varphi)$ is obtained when $\theta = \arcsin \sqrt{\frac{2}{3}}$ and $\varphi = \arcsin \sqrt{\frac{1}{2}}$, which are the angles at the diagonals of a 3D cell. Thus, for any propagation angle, the revised 3D CFL condition is

$$
\Delta t \leq \frac{\Delta x}{c \sqrt[3]{3} \sin \left( \frac{k_{\text{max}} \Delta x}{2 \sqrt[3]{3}} \right)}.
$$

(A.3)
1. The conventional 3D FDTD method with CFLN=1.

2. The 3D filtered FDTD method that applies the low pass filter in both \( E \) and \( H \). DCT technique is used and source is excited in \( E \) field.

3. The 3D filtered FDTD method that applies the low pass filter only in \( E \). DCT technique is used and source is excited in \( E \) field.

4. The 3D filtered FDTD method that applies the low pass filter only in \( H \). DCT technique is used and source is excited in \( E \) field.

<table>
<thead>
<tr>
<th>Scenario</th>
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</tr>
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<tbody>
<tr>
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</tr>
<tr>
<td>3</td>
<td>The 3D filtered FDTD method that applies the low pass filter only in ( E ). DCT technique is used and source is excited in ( E ) field.</td>
</tr>
<tr>
<td>4</td>
<td>The 3D filtered FDTD method that applies the low pass filter only in ( H ). DCT technique is used and source is excited in ( E ) field.</td>
</tr>
</tbody>
</table>

Table A.1: The four scenarios in the numerical experiments in the 3D filtered FDTD method.

The upper limit of \( \Delta t_{cfl} \) is greater than the upper limit of the conventional 3D CFL condition \( \Delta t_{cfl} = \sqrt{3} \Delta x / c \) with a factor of \( 1/\sin \left( \frac{k_{max} \Delta x}{2\sqrt{3}} \right) \).

A.2 3D Filtered FDTD Method

A.2.1 Observed Signals with Single Point Excitation

The computational space of the 3D filtered FDTD method is a 3D cavity which is discretized by \( 200 \times 200 \times 200 \) Yee cells and bounded by PEC. Each Yee cell is a \( 1 \text{ mm } \times 1 \text{ mm } \times 1 \text{ mm } \) cube. Thus the 3D \( \Delta t_{cfl} \) is 1.92 ps. \( E_z \) is excited at \((100,100,100)\) with the source in (5.1). Figure A.1 shows the signals observed at point \((90,100,100)\) for four scenarios, which are defined in Table A.1. Scenario 1 updates the electromagnetic field components by using the conventional FDTD method with CFLN=1. The spatial filtering procedure is applied in scenarios 2, 3 and 4 with CFLN=4. The electromagnetic fields of scenarios 2, 3 and 4 are transformed by the DCT/IDCT technique. All the results in the filtered FDTD method differ from the conventional FDTD method. The discrepancy is caused by the excitation condition. In the 3D FDTD method, the single point excitation generates high spatial frequency components at the beginning of the simulation. However these high spatial frequency components are removed by
Figure A.1: The observed signals at (90,100,100) in $E_z$ for four scenarios. The four scenarios are introduced in Table 5.2. In scenarios 2, 3 and 4, $\tilde{k}_{\text{max}} = 220\pi$ rad/m and CFLN=4.

the filtered FDTD method, which affects the results in the spatial domain. To reduce the impact of the filtered FDTD method on the source excitation, the filtering procedure can be applied after the main pulse of the source is excited. For example, with the excitation shown in Figure 5.1, the filtering procedure can be started at $t = 0.6$ ns. However, when the excitations is longer than the total execution time, the 3D filtered FDTD method with the single point excitation is invalidated. To overcome this drawback, the spherical excitation is introduced into the 3D filtered FDTD method.

**A.2.2 Observed Signals with Spherical Excitation**

The high spatial frequency components generated from the single point excitations can be avoided by smoothing the field distribution around the excitation point. The soft source excitation of the spherical excitation is expressed as

$$E_{z}^{n}(i, j, k) = E_{z}^{n}(i, j, k) - E_{\text{sphere}}(i, j, k)E_{\text{source}}(n\Delta t)$$  \hspace{1cm} (A.4)
where $E_{\text{sphere}}(i,j,k)$ is the shape of the spherical excitation. $E_{\text{sphere}}(i,j,k)$ is defined as

$$E_{\text{sphere}}(i,j,k) = \begin{cases}  
  e^{-\left(\frac{(i-i_{\text{src}})^2 + (j-j_{\text{src}})^2 + (k-k_{\text{src}})^2}{2\tau_{\text{sphere}}^2}\right)}, & \sqrt{(i-i_{\text{src}})^2 + (j-j_{\text{src}})^2 + (k-k_{\text{src}})^2} \leq E_{\text{radius}} \quad (A.5) \\
  0, & \sqrt{(i-i_{\text{src}})^2 + (j-j_{\text{src}})^2 + (k-k_{\text{src}})^2} > E_{\text{radius}} 
\end{cases}$$

where $(i_{\text{src}}, j_{\text{src}}, k_{\text{src}})$ is the center of the spherical excitation, $E_{\text{radius}}$ is the radius of the sphere of the excitation points and $\tau_{\text{sphere}}$ is the parameter that determines the decay of $E_{\text{sphere}}$.

With the spherical excitation of $\tau_{\text{sphere}} = 4$, $E_{\text{radius}}$ is 5 cells and $(i_{\text{src}}, j_{\text{src}}, k_{\text{src}})$ is at $(100, 100, 100)$, Figure A.2 shows the signals observed at $(85,100,100)$ in the conventional FDTD method and filtered FDTD method. Comparing to Figure A.1, the accuracy of the filtered FDTD method is improved as shown in Figure A.2. The observed signal in scenario 2 is identical to the reference signal in scenario 1. In scenarios 3 and 4, the observed signals present a minor difference to the reference. The accuracy of the 3D filtered FDTD method improves when the radius of the spherical excitation increases. In the numerical experiments, to avoid the high spatial frequency generated from the excitation, the radius of the spherical excitation should be at least 3 cells.
A.2.3 Improvement of Computational Efficiency

In the 3D filtered FDTD method with spherical excitation, Figure A.3 compares the maximum CFLN for stable computational in the numerical experiments with the theoretical value. Figure A.3 shows that the maximum stable CFLN for the numerical experiments is higher than the theoretical value. Figure A.4 compares the computational efficiency of only filtering one field (either $E$ or $H$) with two fields (both $E$ and $H$). As demonstrated in Figure A.4 with only one filtered field, the filtered FDTD method is faster than the conventional FDTD method when CFLN is greater than 5. In the scenario with two filtered field, the computational speed of the filtered FDTD method is faster than the conventional FDTD method when CFLN is greater than 9. Thus, for the 3D filtered FDTD method, only filtering one field is recommended since the computational speed of filtering the unstable harmonics in either $E$ or $H$ is twice faster than that of filtering in both $E$ and $H$.

A.2.4 3D Filtered FD-FDTD Method with CFS-PML

A.2.4.1 Observed Signals with Spherical Excitation

The whole computational domain in this experiment is composed of $200 \times 200 \times 200$ Yee cells. The computational domain is terminated in 32 CFS-PML layers. Each
Figure A.4: The improvement of computational efficiency.

<table>
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<td>The filtered 3D FD-FDTD method that applies the low pass filter in $E$ and $H$. DCT technique is used and source is excited in $E$. The thickness of CFS-PML is 32 cells.</td>
</tr>
<tr>
<td>3</td>
<td>The filtered 3D FD-FDTD method that applies the low pass filter only in $E$. DCT technique is used and source is excited in $E$. The thickness of CFS-PML is 32 cells.</td>
</tr>
<tr>
<td>4</td>
<td>The filtered 3D FD-FDTD method that applies the low pass filter only in $H$. DCT technique is used and source is excited in $E$. The thickness of CFS-PML is 32 cells.</td>
</tr>
</tbody>
</table>

Table A.2: The four scenarios in the numerical experiments of the 3D filtered FD-FDTD method with CFS-PML.
Figure A.5: The observed signals at (75,100,100) in $E_z$ for four scenarios. The computational domain is filled with fat. The four scenarios are introduced in Table A.2. In scenarios 2, 3 and 4, $\tilde{k}_{\text{max}} = 220\pi$ rad/m and CFLN=4. The cell is a 1 mm $\times$ 1 mm $\times$ 1 mm cube. The centre of the spherical excitation is at (90,100,100). The spherical excitation is generated by $\tau_{\text{sphere}} = 4$ and $E_{\text{radius}} = 5$.

Figure A.5 shows the signals observed at (75,100,100) in the conventional FDTD method and filtered FDTD method for four scenarios which are introduced in Table A.2. The observed signal in scenario 1 is obtained from the conventional FD-FDTD method with CFLN=1. The observed signals in scenario 2, 3 and 4 are obtained from the filtered FD-FDTD method with CFLN=4. Among the scenarios 2, 3 and 4, only filtering out the high spatial frequencies in the magnetic field presents the best accuracy. Thus, for the 3D filtered FD-FDTD method with CFS-PML, the results are affected by filtering out the high spatial frequency components in the electric field.

A.2.4.2 Improvement of Computational Efficiency

Figure A.6 and Figure A.7 present the extended stability and the speed improvement of the 3D filtered FD-FDTD method by applying low-pass filter only in the magnetic field. Figure A.6 shows that the maximum stable CFLN for the numerical experiments are higher than theoretical value (A.3) when $k_{\text{max}}$ is less than 125$\pi$ rad/m. As shown in Figure A.7, the computational speed of the 3D filtered FDTD method is faster than the conventional FDTD method when CFLN is greater than 9.
The theoretical value

Filtering only $H$

Figure A.6: The maximum CFLN which gives stable computation for each $\tilde{k}_{\text{max}}$. The theoretical value is obtained from (A.3).

Figure A.7: The improvement of computational efficiency.
Bibliography


