Finite-difference time-domain methods for anisotropic media with total-field/scattered-field formulation

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Finite-Difference Time-Domain Methods for Anisotropic Media with Total-Field/Scattered-Field Formulation

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Abstract

Analysis of electromagnetic (EM) wave phenomena in complex media has attracted considerable interest over recent years, particularly due to applications such as biomedical, environmental remote sensing and photonic bandgap. In such applications, EM wave can interact with arbitrary geometries composed of anisotropic, dispersive and inhomogeneous media. In such cases, the use of analytical methods to obtain EM solutions may not be possible, thus, numerical methods that discretize Maxwell's equations on a volumetric mesh are often sought. The finite-difference time-domain (FDTD) method is one such numerical method that is conceptually simple yet robust in handling complex media. However, several intrinsic problems persist, such as the time step size limitation as well as accurate incident wave source. In this research, we investigate such issues in FDTD and propose developments specifically for complex media. Here, the complex media refer to materials that are characterized by anisotropic constitutive relations.

Due to its explicit nature, the FDTD method is subjected to the Courant-Friedrich-Levy (CFL) stability condition that imposes a maximum time step size limitation. This limitation can degrade the computational efficiency of the FDTD method. To overcome the time step size limitation and improve efficiency, several unconditionally stable implicit FDTD methods have been developed, such as the alternating direction implicit (ADI) and split-step FDTD methods. Several efforts have been made to extend implicit FDTD methods for modeling anisotropic media. However, one of the existing challenges is the development of implicit FDTD methods for modeling 3-D wave propagation in general anisotropic media. In this research, a novel implicit split-step FDTD method is presented for treating 3-D wave propagation in general anisotropic media. Stability analysis via the Fourier method along with five different numerical experiments are performed to validate the stability and performance of the proposed method.

The complex-envelope (CE) ADI-FDTD method is a useful implicit FDTD method for modeling anisotropic periodic structures that have very narrow bandwidth resonances and sharp field variations. In this research, extensions of the CE-ADI-FDTD method are presented to treat anisotropic periodic structures composed of ferrite as well as gain media. With magnetic materials, unique electromagnetic effects such as unidirectional wave propagation can be supported. With gain materials such as doped laser dyes in liquid crystals, circularly polarized lasing close to the photonic band edge can be supported. The proposed extensions are formulated based on the efficient ADI-FDTD splitting formulae that can produce simpler and fewer right-hand sides. Numerical validation is performed using examples of magnetic and nonmagnetic photonic crystals.

In the FDTD method, the total-field/scattered-field (TF/SF) formulation is widely used to excite incident waves for scattering analysis of structures that can be anisotropic. An important aspect of the TF/SF formulation is the proper calculation of incident fields based on propagation in discrete FDTD space, instead of continuous physical space. Failure to do so can otherwise result in significant errors. In this research, we present an accurate time-domain analytic method for computing incident fields in the FDTD TF/SF formulation and demonstrate its ability in sourcing both plane wave and focused beam (non-plane wave). The proposed method computes incident fields by using analytic field expressions with higher-order compensations for 1) grid dispersion and 2) frequency-dependent field polarizations. Additional formulations based on Hermite polynomials are presented to facilitate the implementation of the proposed method.

The above research contributions aim to improve both efficiency and accuracy of the FDTD method in modeling EM wave interactions with complex media. It is anticipated that the proposed methods would be useful for analyzing various anisotropic media.

Table of Contents

List of Figures	ix
List of Tables	xiv
List of Abbreviations	xv
1 Introduction	1
1.1 Background and Motivation	1
1.2 Objectives	4
1.3 Major Contributions of Thesis	4
1.4 Organization of The Thesis	6
2 Literature Review	8
2.1 Introduction	8
2.2 FDTD Methods	8
2.2.1 Yee's FDTD Method	8
2.2.2 Alternating Direction Implicit FDTD Method	11

2.2.3	Split-Step FDTD Method	14
2.3	Modeling Anisotropic Media in FDTD	15
2.3.1	Yee's FDTD Method	15
2.3.2	Alternating Direction Implicit FDTD Method	18
2.3.3	Split-step FDTD Method	19
2.4	Modeling Incident Wave Excitations with TF/SF Formulation in FDTD	19
2.4.1	1-D Auxiliary Grid Based Methods	23
2.4.2	Frequency-Domain Analytic Methods	25
2.4.3	Time-Domain Analytic Methods	28
2.5	Concluding Remarks	30
3	Split-Step FDTD Method for General Anisotropic Media	33
3.1	Introduction	33
3.2	Formulation	35
3.2.1	Original Approach	35
3.2.2	Formal Matrix Approach	42
3.2.3	An Extension with PML Boundary Conditions	46
3.3	Stability Analysis	55
3.4	Numerical Results	59
3.4.1	Experiment 1: 3-D Cavity with Homogeneous Anisotropic Media	59
3.4.2	Experiment 2: 3-D Cavity with Anisotropic Dielectric Resonator	64

3.4.3	Experiment 3: 3-D Scattering from Anisotropic Dielectric Cube	67
3.4.4	Experiment 4: 2-D Scattering from Anisotropic Dielectric Cylinder	68
3.4.5	Experiment 5: 2-D Tunable Anisotropic Photonic Crystal Cavity	70
3.5	Concluding Remarks	72
4	Efficient Complex Envelope ADI-FDTD Method for Anisotropic Periodic Media	74
4.1	Introduction	74
4.2	Formulation	77
4.2.1	With Magnetic Media	77
4.2.2	Without Magnetic Media	86
(a)	With Gain	86
(b)	Without Gain	99
4.2.3	An Extension to Two-Dimensional Case	101
4.3	Numerical Results	109
4.3.1	Experiment 1: Magnetic Photonic Crystal	109
4.3.2	Experiment 2: Nonmagnetic Photonic Crystal	114
(a)	With Gain	114
(b)	Without Gain	118
4.3.3	Experiment 3: 2-D Tunable Magnetic Photonic Crystal Cavity .	121

4.4	Concluding Remarks	123
5	Analytic Fields with Higher-Order Compensations for 3-D FDTD TF/SF	
	Formulation	125
5.1	Introduction	125
5.2	FDTD Fourier Analysis	127
5.2.1	Numerical Dispersion	128
5.2.2	Impedance	132
5.2.3	Polarization	133
5.3	Formulation	137
5.3.1	Higher-order Numerical Wavenumber Approximation	137
5.3.2	Frequency-Dependent Field Polarization Compensation	141
5.3.3	Analytic Fields of A Plane Wave with Higher-Order Dispersion and Polarization Compensations	145
5.3.4	Analytic Fields of A Focused Beam with Higher-Order Disper- sion and Polarization Compensations	148
5.4	Computing Derivatives of Gaussian Source Functions	152
5.5	Phase Error Analysis	155
5.6	Numerical Results	157
5.6.1	Experiment 1: Plane Wave Excitation	158
5.6.2	Experiment 2: Focused Beam Excitation	160
5.7	Concluding Remarks	162

6 Conclusion	164
A Computation of Amplification Matrices G_i and G	168
B Coefficients $c_{2,4}^{t,p}$ and $s_{2,4}^{t,p}$	172
C Coefficients $\Delta U_{E,2}$ and $\Delta U_{E,4}$ for Plane Wave Excitation	174
D Coefficients $\Delta U_{E,2}$ and $\Delta U_{E,4}$ for Focused Beam Excitation	176
E Derivation of Recurrence Relations for $g_n^s(t)$ and $g_n^c(t)$	177
References	180
Author's Publication	197

List of Figures

2.1	Electric and magnetic field components positioned in a staggered manner in a 3-D Cartesian grid space.	11
2.2	TF/SF regions of a 3-D FDTD lattice truncated by an ABC. An incident plane wave, propagating in direction $\mathbf{k}_i$, is bounded in the TF region. . .	20
2.3	A 1-D grid with TF/SF boundary defined by $i = is1$ and $i = is2$	21
3.1	Eigenvalues (dots) of amplification matrix $\mathbf{G}$ around unit semicircle for various medium cases.	58
3.2	Example of H_z field update on PEC boundary $z = 0$ in Substep 1.	60
3.3	Time-domain H_z computed using Split-Step FDTD (CFLN=10) and Explicit FDTD for various medium cases.	62
3.4	Resonant frequencies extracted using Split-Step FDTD and Explicit FDTD for case of medium 3 (general anisotropic). Top and bottom plots correspond to resonance at 1.257 GHz and 1.187 GHz, respectively.	63
3.5	Time-domain H_z computed using Split-Step FDTD (CFLN=100) over 80000 iterations for case of medium 3 (general anisotropic).	64

3.6	Magnitude of $E_z(\omega)$ versus frequency computed using Split-Step FDTD (CFLN=5) and Explicit FDTD for case of medium 1 (electric anisotropic dielectric resonator.	66
3.7	Resonant frequencies extracted using Split-Step FDTD and Explicit FDTD for case of anisotropic dielectric resonator. Top and bottom plots correspond to resonance at 6.48×10^8 Hz and 7.78×10^8 Hz, respectively. . .	66
3.8	Time-domain scattered E_y computed using Split-Step FDTD (CFLN=1, 5 and 10) and Explicit FDTD.	67
3.9	Fine-grid staircase mesh of dielectric cylinder.	69
3.10	Radar cross section (dB) computed using Split-Step FDTD (CFLN=1 and 5) and Explicit FDTD.	70
3.11	Normalized resonant frequency versus anisotropy tuning angle ϕ using explicit and split-step (denoted as SS) FDTD methods.	71
3.12	Fine-grid staircase mesh of each cylindrical dielectric rod in PhC cavity (example shown for 1st rod from top-left).	72
3.13	E_z field over PhC for $\phi = 30^\circ$ using split-step FDTD method at CFLN=5. i and j coordinates are in terms of indices while unit of E_z is V/m. . . .	72
4.1	Energy band structure of four-level atomic system.	87
4.2	$N = 16$ periodically stacked array with each unit cell composed of one ferrite layer F and two misaligned anisotropic dielectric layers $A1$ and $A2$.109	
4.3	(a) Band diagram and (b) transmittance plots for lossless magnetic PhC. L is the thickness of a unit cell, $L = L_F + L_{A2} + L_{A1}$. Unit of frequency is Hz.	110

4.4	(a) Band diagram and (b) transmittance plots for lossless <i>nonmagnetic</i> PhC. Ferrite layer F of magnetic PhC is simply replaced by a free space layer. Unit of frequency is Hz.	111
4.5	Normalized $ \mathbf{E} ^2$ versus position for (a) lossless and (b) lossy ferrite cases. Markers $\bigcirc$, $+$ and $\square$ attained with proposed CE-ADI-FDTD method at CFLN of 100, 150 and 200 respectively. Continuous line plot attained with explicit FDTD method at CFLN of 1.	112
4.6	Normalized $ \mathbf{E} ^2$ versus position for (a) lossless and (b) lossy ferrite cases, using proposed CE-ADI-FDTD method at CFLN=200. Continuous and dotted line plots indicate incident field excitation towards the $+z$ and $-z$ directions, respectively.	113
4.7	Simulation of cholesteric liquid crystal (CLC) with gain.	115
4.8	Time-domain plot of electric fields E_x and E_y sampled at observation point in glass substrate.	116
4.9	Steady-state time-domain plot of electric fields E_x and E_y around the time of 5ps.	117
4.10	Plot of transmittance and lasing spectrum.	117
4.11	(a) Transmittance for different incident wave polarizations ϕ_{pol} and (b) band diagram illustrating the split band edges of a SBE PhC with $N = 11$. ϕ_{pol} is the angle between the incident electric field vector and the x axis. L is the thickness of a unit cell, $L = L_{A1} + L_{A2} + L_B$	119

4.12	Time-averaged field intensity $ \mathbf{E} ^2$ of a SBE PhC with $N = 11$ for different incident wave polarizations ϕ_{pol} . Continuous line plots with and without marker $\bigcirc$ represent $ \mathbf{E} ^2$ values obtained using proposed efficient CE-ADI-FDTD method and CE-ADI-FDTD method presented in [64], respectively.	120
4.13	Field intensity achieved inside the SBE PhC for different polarizations matched to a) $\phi_{pol,2} = 0^\circ$ and b) $\phi_{pol,2} = 90^\circ$	121
4.14	Fine-grid meshing of 2-D magnetic PhC.	122
4.15	Variation of 2-D PhC defect mode frequency for different values of external biasing magnetic field $\omega_0 = \omega_{0,c} \frac{2\pi c}{a}$	122
5.1	Plot of $\log_{10} Error = \tilde{k} - \tilde{k}_{3rd/5th} $ versus $\log_{10}(\omega\Delta t)$ for propagation direction of $\phi = 70^\circ$ and $\theta = 30^\circ$	141
5.2	Plot of $\log_{10} Error $ versus $\log_{10}(\omega\Delta t)$. Dash- and dot-lines represent errors from trigonometric function approximations correct to $(\omega\Delta t)^0$ and $(\omega\Delta t)^4$, respectively. 'o', '▷', '◁' and '+' represent errors from $\sin\tilde{\theta}$, $\cos\tilde{\theta}$, $\cos\tilde{\phi}$ and $\sin\tilde{\phi}$ approximations, respectively. Slope of dash- and dot-lines are 2 and 6, respectively.	143
5.3	Plot of $\log_{10}(DotProductError)$ versus $\log_{10}(\omega\Delta t)$	144
5.4	(a) Schematic of a focused beam formed by an aplanatic lens with spherical converging wavefront $\mathbf{w}$ and focus $\mathbf{F}$ at origin and (b) TF/SF formulation that models the focal area of the converging lens.	149
5.5	Comparison between n th derivatives of modulated Gaussian pulse computed via proposed recurrence relations and analytic derivations (denoted with marker +).	155

5.6	Plot of higher-order n th derivatives of modulated Gaussian pulse, computed using the proposed recurrence relations.	155
5.7	Plot of (a) phase errors $ \Theta_{ref} - \Theta_{l,m} $ for fixed $N_\lambda=20$ and (b) phase error $ \Theta_{ref} - \Theta_{5,3} $ for different N_λ values.	157
5.8	Field leakage in the scattered-field region using modulated Gaussian source with $\omega_0 = 5\pi \times 10^9$ rad/s ($N_\lambda = 10$). The field leakage is below -86 dB using the proposed analytic expressions. Lower-order compensation corresponds to dispersion compensation procedure in [91].	158
5.9	Field leakage in the scattered-field region using modulated Gaussian source with $\omega_0 = 2\pi \times 10^9$ rad/s ($N_\lambda = 20$). The field leakage is below -137.3 dB using the proposed analytic expressions. Lower-order compensation corresponds to dispersion compensation procedure in [91].	159
5.10	Grayscale plots of E_x field (in dB) on the $y = 0$ (xz) plane at different time instants (a)-(f). The colorplot bar is restricted to -40 dB.	160
5.11	E_x scattered field leakage (in dB) comparison at grid point (61,61,10) on xy plane, 1 cell below the exit plane of the focused beam.	161
5.12	E_x scattered field leakage (in dB) comparison at grid point (61,61,112) on xy plane, 1 cell above the entrance plane of the focused beam.	162

List of Tables

3.1	Comparison of CPU time between proposed split-step FDTD and explicit FDTD for Experiment 1	62
3.2	Comparison of CPU time between proposed split-step FDTD and explicit FDTD for Experiment 2	65
4.1	Flops count and number of RHS terms comparison between proposed efficient and conventional CE-ADI-FDTD methods	101

List of Abbreviations

ABC	Absorbing Boundary Condition
ADI	Alternating Direction Implicit
AFP	Analytic Field Propagator
CE	Complex Envelope
CFLN	Courant Number
CFL	Courant-Friedrich-Levy
CLC	Cholesteric Liquid Crystal
CPU	Central Processing Unit
DBE	Degenerate Band Edge
DNG	Double-Negative
EM	Electromagnetic
FDTD	Finite-Difference Time-Domain
LOD	Locally 1-D
MAP	Multipoint Auxiliary Source Propagator
PEC	Perfect Electric Conductor
PhC	Photonic Crystal

PML	Perfectly Matched Layer
RCS	Radar Cross Section
RHS	Right-Hand Side
SBE	Split Band Edge
SIP	Stationary Inflection Point
SS	Split-Step
TE	Transverse Electric
TF/SF	Total-Field/Scattered-Field
TM	Transverse Magnetic

Chapter 1

Introduction

1.1 Background and Motivation

Analysis of electromagnetic (EM) wave phenomena in complex media has been a topic of continual interest. Over recent years, several areas of applications have served as catalysts for this interest. Some of these areas are listed as follows:

- (1) Interaction of EM wave with biological tissues in biomedical applications such as noninvasive diagnosis of virus/cancerous cells, medical imaging of tumors and investigating the effects of long term exposure of humans to EM radiation. Biological tissues are, in general, arbitrary configurations of inhomogeneous, lossy and frequency dispersive dielectric materials. These materials can also be anisotropic.
- (2) Interaction of EM wave with earth media in applications such as global climate assessment and environmental remote sensing. Such earth media include soils, vegetation, rocks and snow that can be characterized by anisotropic constitutive relations.

- (3) EM wave interaction with EM engineered materials such as left-handed or double-negative (DNG) metamaterials, photonic bandgap and surface plasmon materials. These engineered materials can have, in general, complex constitutive relations that are inhomogeneous, anisotropic and frequency dispersive. They have been used in devices with unique EM responses from the microwave to optical frequency range.

For such complex media which may be anisotropic, lossy, dispersive and inhomogeneous in arbitrary geometries, the use of analytical methods to obtain EM solutions can be a very complicated task. As a result, numerical methods that discretize Maxwell's equations directly on a volumetric mesh are often sought. The finite-difference time-domain (FDTD) method is one such class of numerical methods that is conceptually simple yet robust in handling complex media and can produce wideband results in a single simulation run. These attributes coupled with the rapid increase in computer memory capacities and visualization capabilities has led to an expansion of interest in the FDTD method amongst researchers and engineers in the general EM community. Despite its advantages, several intrinsic problems still persist when modeling complex media with the FDTD method. These problems include use of staircase approximations when modeling interfaces, use of absorbing boundary conditions for truncating computational domain, implementing incident wave excitations for scattering analysis and overcoming the maximum time step size limitation imposed by the Courant-Friedrich-Levy (CFL) stability condition. In this thesis, we address some of these problems when modeling complex media characterized by anisotropic constitutive relations.

To overcome the CFL stability condition in the explicit FDTD method, several unconditionally stable implicit FDTD methods such as the alternating direction implicit (ADI) and split-step FDTD methods have been developed. These implicit FDTD methods can

be computationally efficient compared to the explicit FDTD method. Several efforts have further been made to extend the implicit FDTD methods to model anisotropic media. However, much of these extensions are limited to the case of 1-D and 3-D wave propagation in anisotropic media characterized by 2-D and diagonal material tensors, respectively. One of these extensions is termed as the complex envelope (CE) ADI-FDTD method and is especially useful for modeling anisotropic periodic structures. The CE-ADI-FDTD method is however unable to accommodate magnetic materials such as ferrites or gain materials. Periodic structures composed of magnetic materials can exhibit unique electromagnetic effects for instance unidirectional wave propagation. Periodic structures, such as laser dye doped cholesteric liquid crystals, can exhibit circularly polarized lasing at the edge of the stop band.

In the FDTD method, the total-field/scattered-field (TF/SF) formulation is widely used to excite incident waves for scattering analysis of structures that can be anisotropic. An important aspect of the TF/SF formulation is the calculation of incident fields based on propagation in discrete FDTD space, instead of continuous physical space. Computing fields based on the latter can result in significant errors. There are generally two methods to compute these incident fields: 1-D auxiliary grid method and frequency-domain as well as time-domain analytic methods. The former method is primarily used to excite a plane wave while the latter analytic methods can be used to excite both plane and non-plane waves. The time-domain analytic method requires lesser memory storage compared to its frequency-domain counterpart, however, it is less accurate. Since the time-domain analytic method can excite both plane and non-plane waves and requires lesser memory storage, it would be useful to improve on its accuracy.

1.2 Objectives

In this research, we aim to further investigate and develop FDTD methods specifically for efficient modeling of anisotropic media with implicit FDTD methods and accurate modeling of incident wave excitations for scattering analysis of structures that can be anisotropic. Given the motivation presented in Section 1.1, the main objectives are as follows:

- (1) To propose a novel implicit FDTD method based on the split-step scheme to efficiently model 3-D wave propagation in general anisotropic media.
- (2) To extend on the existing implicit FDTD method termed as CE-ADI-FDTD method to efficiently analyze anisotropic periodic media composed of magnetic and gain materials.
- (3) To improve the accuracy of time-domain analytic method to excite incident waves in the TF/SF formulation for FDTD scattering analysis of structures that can be anisotropic.

1.3 Major Contributions of Thesis

In this section, we summarize the major contributions of this thesis.

A novel implicit split-step FDTD method is proposed for efficient modeling of 3-D wave propagation in general anisotropic media. Using the proposed splitting approach, an extension to perfectly matched layer boundary conditions is further exemplified. It is anticipated that, by using this proposed splitting approach, further extensions of the

split-step FDTD method can be made to incorporate for example loss and frequency dispersion, in addition to anisotropy. Stability analysis using the Fourier method is presented to illustrate the stable and non-dissipative nature of the proposed method in general anisotropic media. Five numerical experiments are further presented to demonstrate the efficiency of the proposed method in solving both open and closed region problems. This includes an experiment of an anisotropic photonic crystal (PhC) cavity. It is noted that the proposed split-step FDTD method is generally more efficient compared to the explicit FDTD method. This is especially so when the time step size in the split-step FDTD method is more than 4 times the time step size used in the explicit FDTD method.

Four extensions of the implicit CE-ADI-FDTD method are proposed for efficient modeling of anisotropic periodic structures. These four extensions are formulated using an efficient ADI splitting formulae. A CE-ADI-FDTD method is first generally formulated for inhomogeneous media composed of saturated ferrite with loss and anisotropic permittivity tensor. This extension permits the CE-ADI-FDTD method to analyze magnetic PhCs in addition to nonmagnetic PhCs. The CE-ADI-FDTD method is then generally formulated for inhomogeneous media composed of anisotropic permittivity tensor and gain materials. Nonmagnetic PhCs with gain, such as laser dye doped cholesteric liquid crystals, can be efficiently analyzed using this extended CE-ADI-FDTD method. The conventional CE-ADI-FDTD formulation for nonmagnetic PhCs (without gain) is then presented in a more efficient form. Finally a 2-D extension of the CE-ADI-FDTD method is presented for inhomogeneous media with saturated ferrite. This extension can be used to efficiently analyze 2-D magnetic PhC structures. Numerical demonstration of the proposed CE-ADI-FDTD methods are presented using examples of both 1-D and 2-D magnetic and nonmagnetic PhCs. In the demonstration of nonmagnetic PhC, it is further highlighted that the field enhancement effect in the PhC can be optimized for an incident wave polarization by properly tuning the orientation angles of the anisotropy

axes of the PhC layers.

A time-domain analytic method that uses field expressions with higher-order compensations is proposed to compute incident fields in the FDTD TF/SF formulation. The analytic field expressions are presented for both plane wave and focused beam excitations. The higher-order compensations accurately account for grid dispersion and frequency-dependent polarizations, that are identified in the Fourier analysis of FDTD update equations. Using the proposed expressions, errors in the TF/SF formulation can be significantly reduced. To facilitate the implementation of the analytic expressions, additional formulations utilizing Hermite polynomial relations are presented. Numerical experiments are further presented to demonstrate the accuracy of the proposed method in computing incident fields of a 3-D plane wave and focused beam TF/SF source. It is noted that the proposed method is more accurate than existing methods and can attain errors as low as -115.9 dB, for a reasonably discretized grid. The proposed method can thus be used to accurately source incident waves for FDTD scattering analysis of structures that can be anisotropic.

1.4 Organization of The Thesis

Chapter 2 presents a review of several FDTD methods, namely, the explicit Yee's FDTD method and the implicit ADI and split-step FDTD methods. For each of these FDTD methods, a summary of extensions to model anisotropic media along with the TF/SF formulation is presented. Next, Chapters 3 to 5 present the research contributions. Chapter 3 presents a novel implicit split-step FDTD method for 3-D Maxwell's equations in general anisotropic media. The general anisotropic media can be characterized by full permittivity and permeability tensors. Chapter 4 then presents extensions of

the existing implicit complex envelope ADI-FDTD method for modeling anisotropic periodic media. Chapter 5 subsequently presents an accurate time-domain analytic method for computing incident fields in the FDTD TF/SF formulation. Chapter 6 finally summarizes the research contributions of this thesis and provides recommendation for future work.

In this thesis, the complex media is generally referred to materials that are characterized by anisotropic constitutive relations. Chapter 3 considers anisotropic media without loss and without gain. Chapter 4 considers anisotropic media with either gain or loss, modeled via auxiliary differential equations.

Chapter 2

Literature Review

2.1 Introduction

This chapter reviews three major FDTD methods, namely, the explicit Yee's FDTD method, the implicit ADI and split-step FDTD methods in Section 2.2. For each of these FDTD methods, a summary of extensions to model anisotropic media along with the total-field/scattered-field formulation is presented in Sections 2.3 and 2.4, respectively. Section 2.5 concludes the review by identifying several areas for further development.

2.2 FDTD Methods

2.2.1 Yee's FDTD Method

The finite-difference time-domain (FDTD) method was originally conceived by Yee in [1] for Maxwell's equations in an isotropic and non-dispersive medium. In this

method, explicit update equations are formulated in time-domain for the six electric and magnetic field components. These update equations are formed by approximating the space and time derivatives in Maxwell's equations by second order accurate central differences. In this difference scheme, the electric and magnetic field components are positioned in a Cartesian grid space and in a staggered manner, as shown in Fig. 2.1 (Yee's grid). In addition, the field components are sampled in time in a leapfrog manner. This means that all the electric field components are updated and stored at a particular time given the previous values of magnetic field components. Subsequently, all the magnetic field components are computed and stored given the electric field components just updated. The cycle continues again with the update of the electric field components until the time-stepping is completed.

In the Yee's FDTD method, the explicit update equations for the six electric and magnetic field components are as follows:

$$E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} = E_x|_{i+\frac{1}{2},j,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon_{i+\frac{1}{2},j,k}} (H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n - H_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^n) - \frac{\Delta t}{\epsilon_{i+\frac{1}{2},j,k}} (H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n - H_y|_{i+\frac{1}{2},j,k-\frac{1}{2}}^n) \quad (2.1)$$

$$E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} = E_y|_{i,j+\frac{1}{2},k}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon_{i,j+\frac{1}{2},k}} (H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n - H_x|_{i,j+\frac{1}{2},k-\frac{1}{2}}^n) - \frac{\Delta t}{\epsilon_{i,j+\frac{1}{2},k}} (H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n - H_z|_{i-\frac{1}{2},j+\frac{1}{2},k}^n) \quad (2.2)$$

$$E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} = E_z|_{i,j,k+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon_{i,j,k+\frac{1}{2}}} (H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n - H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^n) - \frac{\Delta t}{\epsilon_{i,j,k+\frac{1}{2}}} (H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n - H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^n) \quad (2.3)$$

$$H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} = H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n + \frac{\Delta t}{\mu_{i,j+\frac{1}{2},k+\frac{1}{2}}\Delta z}(E_y|_{i,j+\frac{1}{2},k+1}^{n+\frac{1}{2}} - E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}) - \frac{\Delta t}{\mu_{i,j+\frac{1}{2},k+\frac{1}{2}}\Delta y}(E_z|_{i,j+1,k+\frac{1}{2}}^{n+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}}) \quad (2.4)$$

$$H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+1} = H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n + \frac{\Delta t}{\mu_{i+\frac{1}{2},j,k+\frac{1}{2}}\Delta x}(E_z|_{i+1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}}) - \frac{\Delta t}{\mu_{i+\frac{1}{2},j,k+\frac{1}{2}}\Delta z}(E_x|_{i+\frac{1}{2},j,k+1}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}}) \quad (2.5)$$

$$H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n + \frac{\Delta t}{\mu_{i+\frac{1}{2},j+\frac{1}{2},k}\Delta y}(E_x|_{i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}}) - \frac{\Delta t}{\mu_{i+\frac{1}{2},j+\frac{1}{2},k}\Delta x}(E_y|_{i+1,j+\frac{1}{2},k}^{n+\frac{1}{2}} - E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}), \quad (2.6)$$

where Δx , Δy and Δz are the spatial sizes in the x , y and z directions, respectively. Δt is the time step size. i , j , and k are the spatial indices in the x , y and z directions, respectively. n is the time index. The physical space and time positions of field components, for example $E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}$, is $(x = i\Delta x, y = (j + \frac{1}{2})\Delta y, z = k\Delta z, t = (n + \frac{1}{2})\Delta t)$. From (2.1)-(2.3), the electric field components are updated from previous values of magnetic field components, that are positioned staggered to the electric field components. The material permittivity is sampled at the location of the electric field components, which caters for permittivity variation in space. This also applies to material permeability. From (2.4)-(2.6), the magnetic field components are updated using the electric field components just updated. This update procedure continues until the time-stepping ends.

Due to its explicit nature, the Yee's FDTD method is subjected to the Courant-Friedrich-Levy (CFL) stability condition which imposes a maximum constraint on its time step size. The CFL condition is given by

$$\Delta t \leq \frac{1}{c_{max} \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}} \quad (2.7)$$

Figure 2.1: Electric and magnetic field components positioned in a staggered manner in a 3-D Cartesian grid space.

where c_{max} is the maximum phase velocity of the wave propagation in the medium [3]. From (2.7), it can be deduced that the maximum allowed time step is restricted by the smallest cell size used in the Yee's grid. In certain structures where there are combinations of fine and coarse grids, the time step is always restricted to the size of the fine grids, which can degrade the computational efficiency of the Yee's FDTD method. To overcome this CFL limitation, several unconditionally stable FDTD methods have been proposed and are reviewed in Sections 2.2.2 and 2.2.3.

2.2.2 Alternating Direction Implicit FDTD Method

In Section 2.2.1, it was noted that the Yee's FDTD method, being explicit in nature, suffers from the CFL stability condition that imposes a maximum time step size, depending on the spatial mesh sizes. To overcome the CFL condition, several implicit unconditionally stable FDTD methods have been developed based on techniques such as alter-

nating direction implicit (ADI) [4]-[7], split-step [8]-[10], locally 1-D (LOD) [11]-[14] and Crank-Nicolson [15], [16]. In this section, we present a review of the ADI-FDTD method.

The ADI-FDTD method is a second order accurate implicit scheme both in time and space, with central differencing. The six field components are spatially positioned in a Yee's grid just as in the explicit Yee's FDTD method. However, the electric and magnetic field components are both updated at collocated time steps, instead of half time step apart as in the Yee's FDTD method. The 3-D ADI-FDTD method in isotropic and non-dispersive medium can be written in compact form as

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{A})\mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{B})\mathbf{u}^n \quad (2.8)$$

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{B})\mathbf{u}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{A})\mathbf{u}^{n+\frac{1}{2}} \quad (2.9)$$

where $\mathbf{u} = \begin{bmatrix} E_x & E_y & E_z & H_x & H_y & H_z \end{bmatrix}^T$,

$$\mathbf{A} = \begin{bmatrix} 0 & \epsilon^{-1}\mathbf{D}^T \\ \mu^{-1}\mathbf{D} & 0 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0 & -\epsilon^{-1}\mathbf{D} \\ -\mu^{-1}\mathbf{D}^T & 0 \end{bmatrix} \quad (2.10)$$

and $\mathbf{D} = \begin{bmatrix} 0 & \frac{\partial}{\partial z} & 0 \\ 0 & 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} & 0 & 0 \end{bmatrix}$.

$\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$ and $\frac{\partial}{\partial z}$ are the spatial derivatives in the x , y and z directions, respectively. The entire field update from n to $n+1$ is split into two substeps: n to $n+\frac{1}{2}$ in (2.8) and $n+\frac{1}{2}$ to $n+1$ in (2.9). In each substep, the electric field components (normally electric) are updated first by solving a system of linear equations each, with tridiagonal matrix coefficients. The right-hand sides (RHS) of these systems contain the known electric and

magnetic field terms at previous time steps of n and $n + \frac{1}{2}$ for first and second substep, respectively. Using the solved electric field components, the magnetic field components are then updated explicitly. The ADI-FDTD method has been verified unconditionally stable in [7], [17].

The ADI-FDTD method can permit time step sizes larger than the Courant-limit time step size, that is used in the conventional Yee's FDTD method. As such, fewer iterations may be needed with the ADI-FDTD method, in comparison with the Yee's FDTD method. Hence, the ADI-FDTD method can be more efficient than the Yee's FDTD method with efficiency improving as time step size increases. However, the trade-off is an increase in truncation and numerical dispersion errors [18]-[21]. Some efforts in the form of iterative procedures [22], [23] and parameter optimization [24] have been presented to reduce these errors.

In [25], [26], a more efficient form of the ADI-FDTD method was presented as

$$\mathbf{v}^n = \tilde{\mathbf{u}}^n - \mathbf{v}^{n-\frac{1}{2}} \quad (2.11)$$

$$\left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{A}\right)\tilde{\mathbf{u}}^{n+\frac{1}{2}} = \mathbf{v}^n \quad (2.12)$$

$$\mathbf{v}^{n+\frac{1}{2}} = \tilde{\mathbf{u}}^{n+\frac{1}{2}} - \mathbf{v}^n \quad (2.13)$$

$$\left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{B}\right)\tilde{\mathbf{u}}^{n+1} = \mathbf{v}^{n+\frac{1}{2}} \quad (2.14)$$

with input $\tilde{\mathbf{u}}^n = 2\mathbf{u}^n$ and output $\mathbf{u}^{n+1} = \frac{1}{2}\tilde{\mathbf{u}}^{n+1}$. The set of equations (2.11)-(2.14) are termed as the *fundamental* ADI splitting formulae. Equations (2.11)-(2.12) and (2.13)-(2.14) can be treated as the first and second substeps, respectively, much like the conventional ADI-FDTD method. In each substep however, two sets of updating are performed: auxiliary field updating and intermediate/final field updating via implicit/explicit equations. More importantly, it can be seen that the RHSs of intermediate/final field update

procedures (2.12) and (2.14) are of simplest matrix-operator-free form (resulting in the term *fundamental*). This produces update equations that are much more simpler, easier and efficient to implement compared to the conventional ADI-FDTD method. The use of auxiliary updating (2.11) and (2.13) aids this simplification, without the need for auxiliary memory.

2.2.3 Split-Step FDTD Method

The split-step (SS1) FDTD method [8]-[10] is another implicit unconditionally stable FDTD method. A similar implicit FDTD scheme is the locally 1-D (LOD) FDTD method [11]-[14]. The split-step FDTD method is second order accurate in space with central differencing but first order accurate in time, due to a noncommutativity error term which is not present in the ADI-FDTD method. The six field components are also spatially positioned in a Yee's grid. However, the electric and magnetic field components are both updated at collocated time steps, instead of half time step apart. The 3-D split-step FDTD method in isotropic and non-dispersive medium can be written in compact form as

$$(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{A}) \mathbf{u}^n \quad (2.15)$$

$$(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B}) \mathbf{u}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{B}) \mathbf{u}^{n+\frac{1}{2}} \quad (2.16)$$

where $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{D}$ matrices are given in (2.10). Much like the ADI-FDTD method, the entire field update is split into two substeps and upon expansion of each substep, the fields can be implicitly determined via the solution of a linear system of equations with tridiagonal matrix coefficient. The efficient fundamental form of the split-step FDTD method with RHSs being matrix-free has been presented in [26].

An advantage of the split-step scheme over the ADI scheme is that it is more efficient [11]. However, the drawback is that the temporal accuracy reduces to first order when $\mathbf{A}$ and $\mathbf{B}$ do not commute. To increase the temporal accuracy to second order, a three stage Strang splitting [26] can be performed as

$$(\mathbf{I} - \frac{\Delta t}{4}\mathbf{A})\mathbf{u}^{n+\frac{1}{4}} = (\mathbf{I} + \frac{\Delta t}{4}\mathbf{A})\mathbf{u}^n \quad (2.17)$$

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{B})\mathbf{u}^{n+\frac{3}{4}} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{B})\mathbf{u}^{n+\frac{1}{4}} \quad (2.18)$$

$$(\mathbf{I} - \frac{\Delta t}{4}\mathbf{A})\mathbf{u}^{n+1} = (\mathbf{I} + \frac{\Delta t}{4}\mathbf{A})\mathbf{u}^{n+\frac{3}{4}}. \quad (2.19)$$

From (2.17)-(2.19), we can deduce that this three stage splitting incurs some additional computational cost compared to the two stage splitting in ADI-FDTD method, to preserve the second order accuracy. An alternative second order accurate two stage splitting scheme has been presented in [12] in the form of the LOD-FDTD method.

2.3 Modeling Anisotropic Media in FDTD

2.3.1 Yee's FDTD Method

The Yee's FDTD method was initially extended in [27] for treating diagonal anisotropic media. In this extension, the isotropic material terms in the field update equations were simply replaced with corresponding diagonal terms of the material tensors. An extension to anisotropic materials with full permittivity and conductivity tensors was subsequently presented in [28]. By including anisotropic permeability, the method in [28] can

be generally expressed in compact form as [29]

$$\mathbf{E}^{n+\frac{1}{2}} = \left(\frac{\bar{\bar{\epsilon}}}{\Delta t} + \frac{\bar{\bar{\sigma}}}{2} \right)^{-1} \cdot \left[\left(\frac{\bar{\bar{\epsilon}}}{\Delta t} - \frac{\bar{\bar{\sigma}}}{2} \right) \cdot \mathbf{E}^{n-\frac{1}{2}} + \nabla \times \mathbf{H}^n \right] \quad (2.20)$$

$$\mathbf{H}^{n+1} = \mathbf{H}^n - \Delta t \bar{\bar{\mu}}^{-1} \cdot \nabla \times \mathbf{E}^{n+\frac{1}{2}}, \quad (2.21)$$

where $\bar{\bar{\epsilon}}$, $\bar{\bar{\mu}}$ and $\bar{\bar{\sigma}}$ are the permittivity, permeability and conductivity tensors, respectively. The field components in (2.20)-(2.21) can be spatially discretized onto the staggered Yee's grid with the spatial derivatives approximated using second order accurate central differences [28]. However, a consequence is that the field components associated with the off-diagonal terms are not directly available from the Yee's grid and have to be interpolated from neighboring grid points.

To clarify, consider a 2-D Yee's grid with the field components $E_x|_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$, $E_y|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}$ and $H_z|_{i+\frac{1}{2},j+\frac{1}{2}}^{n+1}$. The medium is assumed lossless and homogeneous with an isotropic permeability μ and anisotropic permittivity $\bar{\bar{\epsilon}}$. Such a medium can be referred to as electric anisotropic. The inverse of $\bar{\bar{\epsilon}}$ is represented by the impermittivity tensor $\bar{\bar{\kappa}} = \bar{\bar{\epsilon}}^{-1}$. For this 2-D case, the update equations (2.20)-(2.21) with field components spatially discretized onto the Yee's grid are

$$E_x|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = E_x|_{i+\frac{1}{2},j}^{n-\frac{1}{2}} + \frac{\Delta t \kappa_{xx}}{\Delta y} (H_z|_{i+\frac{1}{2},j+\frac{1}{2}}^n - H_z|_{i+\frac{1}{2},j-\frac{1}{2}}^n) - \frac{\Delta t \kappa_{xy}}{\Delta x} (H_z|_{i+1,j}^n - H_z|_{i,j}^n) \quad (2.22)$$

$$E_y|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = E_y|_{i,j+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t \kappa_{yx}}{\Delta y} (H_z|_{i,j+1}^n - H_z|_{i,j}^n) - \frac{\Delta t \kappa_{yy}}{\Delta x} (H_z|_{i+\frac{1}{2},j+\frac{1}{2}}^n - H_z|_{i-\frac{1}{2},j+\frac{1}{2}}^n) \quad (2.23)$$

$$H_z|_{i+\frac{1}{2},j+\frac{1}{2}}^{n+1} = H_z|_{i+\frac{1}{2},j+\frac{1}{2}}^n + \frac{\Delta t}{\mu \Delta y} (E_x|_{i+\frac{1}{2},j+1}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j}^{n+\frac{1}{2}}) - \frac{\Delta t}{\mu \Delta x} (E_y|_{i+1,j+\frac{1}{2}}^{n+\frac{1}{2}} - E_y|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}), \quad (2.24)$$

where κ_{xx} , κ_{xy} , κ_{yx} and κ_{yy} are elements of $\bar{\kappa}$. In (2.22)-(2.23), the field components $H_z|_{i,j}^n$, $H_z|_{i+1,j}^n$ and $H_z|_{i,j+1}^n$ are not directly available from the Yee's grid. These components correspond to the off-diagonal elements κ_{xy} and κ_{yx} . They can be attained by interpolation from four values in the neighboring grid points as [28], [30]

$$H_z|_{i,j}^n = \frac{1}{4}(H_z|_{i+\frac{1}{2},j+\frac{1}{2}}^n + H_z|_{i+\frac{1}{2},j-\frac{1}{2}}^n + H_z|_{i-\frac{1}{2},j+\frac{1}{2}}^n + H_z|_{i-\frac{1}{2},j-\frac{1}{2}}^n). \quad (2.25)$$

Several extensions of the above method were presented in [31] in the form of higher-order approximations of spatial derivatives and interpolation terms as well as alternate grid structures. These alternate grids include either collocating all electric and magnetic field components at a common point or collocating the electric and magnetic field components at two different points separated by half cell space. An immediate advantage of such a grid system is that interpolations such as (2.25) need not be performed. Such alternate grids can result in varying numerical dispersion characteristics [32] and may require additional memory and computational requirements [31]. An alternate FDTD method in terms of $\mathbf{D}$ (electric flux), $\mathbf{E}$ and $\mathbf{H}$ fields was presented in [33], specifically for treating perfect electric conductor (PEC) boundary conditions. Further extension of this method to include $\mathbf{B}$ (magnetic flux) was presented in [34]. In [35], an explicit FDTD method in 3-D cylindrical grids was presented to model full anisotropic conductive media.

Several efforts have also been made to treat materials that are both anisotropic and frequency dispersive with the explicit FDTD method [34], [36]-[53]. These include the treatment of magnetized plasma [36]-[41], ferrites [34], [42]-[48], anisotropic frequency-dispersive metamaterials [49]-[50] and electromagnetic wave cloaking devices [51]-[54]. The dispersive nature is generally treated by methods such as auxiliary differential equations, piecewise linear recursive convolution and exponential time differencing. Various

developments have also been made to model the truncation of an anisotropic media with perfectly matched layer (PML) absorbing boundary conditions [55]-[59].

2.3.2 Alternating Direction Implicit FDTD Method

Several developments have also been made to extend the implicit ADI-FDTD method for modeling anisotropic media. Materials with diagonal permittivity tensor have been analyzed by the ADI-FDTD method [60]. PML absorbers characterized by diagonal material tensors have also been implemented in the ADI-FDTD [61]-[62].

The ADI-FDTD method, in a complex-envelope (CE) formulation, has further been used to analyze periodic structures with unit cells composed of layers of anisotropic dielectrics [63]-[66]. The anisotropic dielectrics are characterized by 2-D permittivity tensors with anisotropy in the xy plane. Generally, for such periodic structures, very fine meshing is required to capture sharp field variations. This requirement, coupled with the Courant stability condition, results in very fine temporal resolutions in the conventional FDTD method. In addition, these structures can require very long simulation times to allow for narrowband resonances to reach steady-state. The fine temporal resolution along with long simulation times thus results in significant number of temporal iterations in the conventional FDTD method. By allowing for larger time step sizes with the ADI-FDTD method, the number of temporal iterations can be reduced. The CE-ADI-FDTD method further permits even larger time step sizes, without compromising accuracy. This is because the numerical dispersion error in the CE formulation [67]-[70] is dependent on the source bandwidth instead of the maximum frequency [63]. Thus, for structures with very narrowband resonances (such as the periodic structures considered in [63]-[65]), low dispersion errors can be achieved even at large Courant numbers [68]. Extensions of the CE-ADI-FDTD method to model anisotropic dielectrics with loss have been made

in [66].

2.3.3 Split-step FDTD Method

Several developments have also been made to extend the implicit split-step FDTD method for modeling anisotropic media, specifically in the form of PML absorbers characterized by diagonal material tensors [71].

2.4 Modeling Incident Wave Excitations with TF/SF Formulation in FDTD

The total-field/scattered-field (TF/SF) formulation [2], [72]-[74] is widely used in the Yee's FDTD method to source incident waves for scattering analysis of structures that can be anisotropic in nature [54], [75]. The TF/SF formulation zones the entire FDTD lattice into two distinct regions, namely, the total-field (TF) and scattered-field (SF) regions. In the TF region (inner zone), the FDTD algorithm operates on total-fields which include both the incident and scattered fields. The interacting structure/scatterer is embedded within this region. In the SF region (outer zone), the FDTD algorithm operates *only* on the outgoing scattered-fields. The boundary separating the TF and SF regions is defined as the TF/SF boundary. The outer lattice planes bounding the SF region, truncates the FDTD lattice with absorbing boundary conditions. Fig. 2.2 illustrates the TF/SF regions of a 3-D FDTD lattice, in which an incident plane wave, propagating in direction $\mathbf{k}_i$, is bounded in the TF region.

Figure 2.2: TF/SF regions of a 3-D FDTD lattice truncated by an ABC. An incident plane wave, propagating in direction $\mathbf{k}_i$, is bounded in the TF region.

To properly connect the TF and SF regions, corrections in terms of incident fields are applied to the field components tangential to the TF/SF boundary. These field corrections serve to correct the inconsistency in the update equations that take the spatial difference between fields in two different regions: the TF and SF regions. For illustration, consider a homogeneous 1-D grid with field components $E_y|_i^{n+\frac{1}{2}}$ and $H_z|_{i+\frac{1}{2}}^{n+1}$. The TF/SF boundary is defined by $i = is1$ and $i = is2$, as shown in Fig. 2.3. The field components that lie on and inside the TF/SF boundary ($is1 \leq i \leq is2$) are the total-fields while those that lie outside the TF/SF boundary ($i < is1$ and $i > is2$) are the scattered-fields. The field components $E_y|_i^{n+\frac{1}{2}}$ and $H_z|_{i+\frac{1}{2}}^{n+1}$ are generally updated using

$$E_y|_i^{n+\frac{1}{2}} = E_y|_i^{n-\frac{1}{2}} - \frac{\Delta t}{\epsilon \Delta x} (H_z|_{i+\frac{1}{2}}^n - H_z|_{i-\frac{1}{2}}^n) \quad (2.26)$$

$$H_z|_{i+\frac{1}{2}}^{n+1} = H_z|_{i+\frac{1}{2}}^n - \frac{\Delta t}{\mu \Delta x} (E_y|_{i+1}^{n+\frac{1}{2}} - E_y|_i^{n+\frac{1}{2}}). \quad (2.27)$$

Update equations (2.26) and (2.27) are consistent for the total-field and scattered-field components in the regions $\{is1 < i < is2\}$ and $\{i \leq is1 - 1 \text{ and } i \geq is2 + 1\}$, respectively. Hence, no field corrections are required for update equations in these regions.

Figure 2.3: A 1-D grid with TF/SF boundary defined by $i = is1$ and $i = is2$.

However, consider the update of field components $E_y^{tot}|_{is1}^{n+\frac{1}{2}}$ and $H_z^{scat}|_{is1-\frac{1}{2}}^{n+1}$ at the left TF/SF boundary at $i = is1$. Applying (2.26) and (2.27) yields,

$$E_y^{tot}|_{is1}^{n+\frac{1}{2}} = E_y^{tot}|_{is1}^{n-\frac{1}{2}} - \frac{\Delta t}{\epsilon \Delta x} (H_z^{tot}|_{is1+\frac{1}{2}}^n - H_z^{scat}|_{is1-\frac{1}{2}}^n) \quad (2.28)$$

$$H_z^{scat}|_{is1-\frac{1}{2}}^{n+1} = H_z^{scat}|_{is1-\frac{1}{2}}^n - \frac{\Delta t}{\mu \Delta x} (E_y^{tot}|_{is1}^{n+\frac{1}{2}} - E_y^{scat}|_{is1-1}^{n+\frac{1}{2}}), \quad (2.29)$$

with superscripts *tot* and *scat* denoting total-field and scattered-field components, respectively. Update equations (2.28) and (2.29) are deemed inconsistent since they involve spatial differences between fields in two different regions.

To overcome this inconsistency, we simply add a correction term each to (2.28) and (2.29) with the correction term being a function of the assumed-known incident field, denoted as superscript *inc*,

$$E_y^{tot}|_{is1}^{n+\frac{1}{2}} = E_y^{tot}|_{is1}^{n-\frac{1}{2}} - \frac{\Delta t}{\epsilon \Delta x} (H_z^{tot}|_{is1+\frac{1}{2}}^n - H_z^{scat}|_{is1-\frac{1}{2}}^n) + \frac{\Delta t}{\epsilon \Delta x} H_z^{inc}|_{is1-\frac{1}{2}}^n \quad (2.30)$$

$$H_z^{scat}|_{is1-\frac{1}{2}}^{n+1} = H_z^{scat}|_{is1-\frac{1}{2}}^n - \frac{\Delta t}{\mu \Delta x} (E_y^{tot}|_{is1}^{n+\frac{1}{2}} - E_y^{scat}|_{is1-1}^{n+\frac{1}{2}}) + \frac{\Delta t}{\mu \Delta x} E_y^{inc}|_{is1}^{n+\frac{1}{2}}, \quad (2.31)$$

since

$$-H_z^{scat}|_{is1-\frac{1}{2}}^n - H_z^{inc}|_{is1-\frac{1}{2}}^n = -H_z^{tot}|_{is1-\frac{1}{2}}^n \quad (2.32)$$

and

$$E_y^{tot}|_{is1}^{n+\frac{1}{2}} - E_y^{inc}|_{is1}^{n+\frac{1}{2}} = E_y^{scat}|_{is1}^{n+\frac{1}{2}}. \quad (2.33)$$

The update equations (2.30) and (2.31) are corrected using the incident field components $H_z^{inc}|_{is1-\frac{1}{2}}^n$ and $E_y^{inc}|_{is1}^{n+\frac{1}{2}}$, respectively. In fact, the incident field information in these correction terms serve to inject and bound the incident wave in the TF region. Similar field corrections can be performed at the right TF/SF boundary at $i = is2$. In this 1-D illustration, 2 tangential incident field components are required each on the left and right TF/SF boundary. For a general 3-D problem, 4 tangential incident field components are required on each side of a cubic TF/SF boundary. Their expressions are presented in detail in [2].

An advantage of the TF/SF formulation is that it provides both scattered-field and total-field results within a single simulation run. The scattered-field results can then be used to attain the far-field response. In addition, the TF/SF formulation is capable of exciting arbitrary incident waves, by simply specifying the incident field values at the boundary between the scattered-field and total-field regions. An important aspect of the TF/SF formulation however is the accurate calculation of the incident fields at the TF/SF boundary. A direct approach to compute these incident fields is to use analytic closed form expressions (e.g sinusoids and exponentials) that describe the space-time behaviour of the incident wave in continuous space [2]. Such analytic expressions do not however capture the manner in which the incident wave actually propagates in a discretized FDTD grid. This mismatch can result in errors such as field leakages from the TF into the SF region. Recently, several methods have been developed to reduce this numerical mismatch [76]-[92]. These methods can generally be categorized as 1-D auxiliary grid based methods [76]-[85] as well as frequency-domain [86]-[90] and

time-domain [91], [92] analytic based methods. In the following subsections, we review some popular methods from each of these categories.

2.4.1 1-D Auxiliary Grid Based Methods

An efficient method to obtain the required incident fields at the TF/SF boundary, specifically for a plane wave, is to interpolate them from similar fields in an auxiliary 1-D FDTD grid [2]. The 1-D grid points in the direction of propagation of the incident plane wave and is updated along with the main grid with same spatial and time step sizes. Despite its efficiency, the accuracy of the 1-D grid method is limited for *non-grid* aligned propagations due to numerical mismatch between the auxiliary 1-D FDTD mesh and the main FDTD mesh in terms of phase velocities and field locations as well as polarizations. To ameliorate this numerical mismatch, several developments of the 1-D grid method have been proposed, namely in the form of higher-order interpolations [76], finer 1-D grid sampling as well as signal-processing techniques [77] and spatial step size optimizations for phase velocity matching over a wide frequency band [78].

Recently, a new 1-D grid method termed as 1-D Multipoint Auxiliary Source Propagator (MAP) was proposed in [79] to source the TF/SF boundary in a 2-D main grid for a discrete set of propagation angles called the rational angles. The 1-D MAP approach produces a dispersion relation identical to that of the main grid at the rational angles and maps the field values to the TF/SF boundary with no interpolation. This method results in a low field leakage error of less than -300 dB. To illustrate this method, consider sourcing a plane wave into a 2-D TM_z main grid. The plane wave is propagating in direction ϕ with respect to the x axis. An auxiliary 1-D MAP grid is used to propagate

the electric field. The update equation for this 1-D MAP grid is

$$e_z|_i^{n+1} = -e_z|_i^{n-1} + 2(1 - S_x^2 - S_y^2)e_z|_i^n + S_x^2(e_z|_{i+m_x}^n + e_z|_{i-m_x}^n) + S_y^2(e_z|_{i+m_y}^n + e_z|_{i-m_y}^n), \quad (2.34)$$

where $S_\xi = \frac{c\Delta t}{\Delta \xi}$ for $\xi = x, y$ and $m_{x,y}$ are integers. The 1-D MAP grid has time step size Δt , similar to that of the main grid. The spatial distance between e_z field points in the 1-D grid is Δr . The dispersion relation produced by this update equation is

$$\frac{S_x^2 \sin^2(\frac{\tilde{k}m_x\Delta r}{2})}{\sin^2(\frac{\omega\Delta t}{2})} + \frac{S_y^2 \sin^2(\frac{\tilde{k}m_y\Delta r}{2})}{\sin^2(\frac{\omega\Delta t}{2})} = 1. \quad (2.35)$$

This dispersion relation is identical to that of a 2-D main grid (see (2.41)) when

$$m_x\Delta r = \cos\phi\Delta x \quad \text{and} \quad m_y\Delta r = \sin\phi\Delta y. \quad (2.36)$$

or

$$\Delta r = \frac{\cos\phi\Delta x}{m_x} = \frac{\sin\phi\Delta y}{m_y}. \quad (2.37)$$

From (2.37), it is noted that to match the dispersion relation of the 1-D MAP grid to that of the main grid, the propagation direction angles are restricted to

$$\tan\phi = \frac{m_y\Delta x}{m_x\Delta y}. \quad (2.38)$$

These propagation angles are termed rational angles. In theory, any propagation angle can be satisfied by allowing larger integers of $m_{x,y}$, which implies that Δr is smaller.

Extensions of the 1-D MAP method to source 3-D plane wave have been made in the form of a hybrid time-frequency domain technique in [80] and a time-domain technique in [81]. The memory storage requirement for the 3-D case [81] is $O([m_x + m_y + m_z]N)$ where $m_{x,y,z}$ are integers that depend on the desired resolution of the rational angle and N is the dimension of a side of a cubic TF/SF boundary. If a rational angle is selected such that $[m_x + m_y + m_z] < N$, the 1-D MAP method requires lesser memory storage compared to analytic methods ($O(N^2)$). However, if a fine angular resolution is desired, the term $[m_x + m_y + m_z]$ can be larger than N . The computational requirement of the 1-D MAP then becomes comparable or possibly larger than that of the analytic method.

2.4.2 Frequency-Domain Analytic Methods

An alternate method for plane wave source excitation was presented in [86], in which the incident fields at the TF/SF boundary are directly calculated by analytical means that account for 1) the FDTD numerical dispersion and 2) the non-orthogonality between the frequency-dependent field polarizations and the wavevector [93]. This method called Analytic Field Propagator (AFP) first computes the incident fields in frequency-domain for each point at the TF/SF boundary given the field at a reference point, the direction of propagation and the dispersion relation. An inverse Fourier transform is then performed to obtain the time sequences of the incident fields at the TF/SF boundary. As an illustration, consider sourcing a plane wave into a 2-D TM_z grid. The TM_z fields along with their space-time positions are $E_z|_{i,j}^n$, $H_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}$ and $H_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$. The plane wave is propagating in direction ϕ with respect to the x axis.

Let $g(n\Delta t)$ be the time-series of the incident field component $E_z|_{i,j}^n$ at a grid reference point (i_{ref}, j_{ref}) . In the frequency domain, the phasor field component $\check{E}_z|_{i,j}$ at any other

point (i, j) in the grid is simply

$$\check{E}_z|_{i,j} = P(i - i_{ref}, j - j_{ref})\mathcal{F}(g) \quad (2.39)$$

where $\mathcal{F}$ is the discrete Fourier transform and complex-valued propagator P is given as

$$P(i - i_{ref}, j - j_{ref}) = e^{-j(\tilde{k}_x(i - i_{ref})\Delta x + \tilde{k}_y(j - j_{ref})\Delta y)}. \quad (2.40)$$

To include FDTD dispersion effects, P uses the numerical wavevector components $\tilde{k}_x$ and $\tilde{k}_y$ that are related through the 2-D FDTD dispersion relation [2]

$$\frac{S_x^2 \sin^2(\frac{\tilde{k}_x \Delta x}{2})}{\sin^2(\frac{\omega \Delta t}{2})} + \frac{S_y^2 \sin^2(\frac{\tilde{k}_y \Delta y}{2})}{\sin^2(\frac{\omega \Delta t}{2})} = 1, \quad (2.41)$$

where $S_\xi = \frac{c\Delta t}{\Delta \xi}$ for $\xi = x, y$. $\tilde{k}_x$ and $\tilde{k}_y$ are components of the numerical wavevector $\tilde{\mathbf{k}} = \tilde{k}\mathbf{U}_k$ with $\mathbf{U}_k = \cos\phi\hat{x} + \sin\phi\hat{y}$. In time-domain, $E_z|_{i,j}^n$ can be attained as

$$E_z|_{i,j}^n = \mathcal{F}^{-1}[P(i - i_{ref}, j - j_{ref})\mathcal{F}(g)] \quad (2.42)$$

where $\mathcal{F}^{-1}$ is the inverse Fourier transform. The magnetic field components can be written in the time-domain as

$$H_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \mathcal{F}^{-1} \left[\frac{S_y \sin(\frac{\tilde{k}_y \Delta y}{2})}{\sin(\frac{\omega \Delta t}{2})} \frac{P(i - i_{ref}, j + \frac{1}{2} - j_{ref})\mathcal{F}(g)}{\eta} \right] \quad (2.43)$$

$$H_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \mathcal{F}^{-1} \left[-\frac{S_x \sin(\frac{\tilde{k}_x \Delta x}{2})}{\sin(\frac{\omega \Delta t}{2})} \frac{P(i + \frac{1}{2} - i_{ref}, j - j_{ref})\mathcal{F}(g)}{\eta} \right] \quad (2.44)$$

where $\eta = \sqrt{\frac{\mu}{\epsilon}}$ is the wave impedance. In (2.43)-(2.44), the terms $\frac{S_y \sin(\frac{\tilde{k}_y \Delta y}{2})}{\sin(\frac{\omega \Delta t}{2})}$ and $-\frac{S_x \sin(\frac{\tilde{k}_x \Delta x}{2})}{\sin(\frac{\omega \Delta t}{2})}$ are related to the FDTD magnetic field polarization with unit vector [85]

$$\mathbf{U}_{\hat{H}} = \begin{bmatrix} \sin \tilde{\phi} \\ -\cos \tilde{\phi} \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{S_y \sin(\frac{\tilde{k}_y \Delta y}{2})}{\sin(\frac{\omega \Delta t}{2})} \\ -\frac{S_x \sin(\frac{\tilde{k}_x \Delta x}{2})}{\sin(\frac{\omega \Delta t}{2})} \\ 0 \end{bmatrix}. \quad (2.45)$$

In general, $\mathbf{U}_{\hat{H}}$ is not equal to the physical magnetic field polarization vector $\begin{bmatrix} \sin \phi \\ -\cos \phi \\ 0 \end{bmatrix}$ and it is not orthogonal to the physical wavevector. In addition, the vector $\mathbf{U}_{\hat{H}}$ is frequency-dependent. Expressions (2.42), (2.43) and (2.44) can be used to accurately compute the required incident fields at the TF/SF boundary. Using the AFP method, the field leakage error can be reduced to levels as low as -180 dB.

Several efforts have also been made to extend the AFP method for FDTD problems with planar interfaces [87], [88]. A similar approach was presented for FDTD problems with layered anisotropic media [89]. In addition to a plane wave, the frequency-domain analytic methods can potentially be used to excite non-plane waves (e.g focused beams) as well. In [90], an approach was outlined, very much similar to the AFP method, to incorporate FDTD numerical effects into each plane wave constituent of a Maxwellian beam. Despite these advantages, a drawback of the frequency-domain analytic methods is that it uses inverse Fourier transforms that can require significant amount of memory ($O(N^2 \times N_t)$) where N_t is number of time steps) to store the incident fields prior to the start of FDTD simulation. This computational requirement becomes a barrier especially for 3-D problems.

2.4.3 Time-Domain Analytic Methods

As presented in Section 2.4.2, a drawback of frequency-domain analytic methods is that it requires significant amount of memory to store incident fields prior to the start of FDTD simulation. This storage requirement can be avoided by utilizing time-domain analytic methods such as [91] and [92].

In [91], the required incident fields at the TF/SF boundary are calculated using analytic expressions that *compensate* for FDTD dispersion in time-domain. We illustrate the method in [91] by considering plane wave excitation into a 3-D FDTD grid. First, consider the 3-D FDTD dispersion relation given as [2]

$$\frac{S_x^2 \sin^2(\frac{\tilde{k}_x \Delta x}{2})}{\sin^2(\frac{\omega \Delta t}{2})} + \frac{S_y^2 \sin^2(\frac{\tilde{k}_y \Delta y}{2})}{\sin^2(\frac{\omega \Delta t}{2})} + \frac{S_z^2 \sin^2(\frac{\tilde{k}_z \Delta z}{2})}{\sin^2(\frac{\omega \Delta t}{2})} = 1, \quad (2.46)$$

where $S_\xi = \frac{c \Delta t}{\Delta \xi}$ for $\xi = x, y, z$ and $\tilde{k}_x, \tilde{k}_y$ and $\tilde{k}_z$ are components of the numerical wavevector $\tilde{\mathbf{k}} = \tilde{k} \mathbf{U}_k$ with $\mathbf{U}_k = \cos \phi \sin \theta \hat{x} + \sin \phi \sin \theta \hat{y} + \cos \theta \hat{z}$. From (2.46), an expression for the numerical wavenumber correct to $(\omega \Delta t)^3$ using series expansions for $\sin^2(x)$ can be attained as

$$\tilde{k} = k_0 + \Delta k \quad (2.47)$$

where

$$\Delta k = \frac{\omega^3}{24} \left(\frac{P_2}{c^3} - \frac{\Delta t^2}{c} \right) + O(\omega^5) \quad (2.48)$$

and

$$P_2 = \Delta x^2 \cos^4 \phi \sin^4 \theta + \Delta y^2 \sin^4 \phi \sin^4 \theta + \Delta z^2 \cos^4 \theta.$$

$k_0 = \frac{\omega}{c}$ is the physical wavenumber. Equation (2.48) can be viewed as an approximate deviation of the numerical wavenumber $\tilde{k}$ from the physical wavenumber k_0 . This deviation is both frequency and propagation direction dependent.

For a plane wave, the incident field at a distance $\mathbf{r}_{i,j,k} = i\Delta x\hat{x} + j\Delta y\hat{y} + k\Delta z\hat{z}$ from a reference point propagates according to

$$\hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, \omega) = \hat{\mathbf{E}}^{ref}(\omega) e^{j\omega t - j(k_0 + \Delta k)\mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}. \quad (2.49)$$

Assuming that $\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}$ is a small quantity, (2.49) is then written as

$$\hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, \omega) \approx (1 - j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}) \hat{\mathbf{E}}^{ref}(\omega) e^{j\omega t - jk_0 \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}. \quad (2.50)$$

Δk in (2.48) is then substituted into (2.50) to yield

$$\begin{aligned} \hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, \omega) \approx & (1 + (j\omega)^3 \frac{\mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}{24c} (\frac{P_2}{c^2} - \Delta t^2)) \\ & \cdot \hat{\mathbf{E}}^{ref}(\omega) e^{j\omega t - jk_0 \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}} \end{aligned} \quad (2.51)$$

Using the Fourier transform identities $(j\omega)^m \leftrightarrow \frac{\partial^m}{\partial t^m}$ and $X(\omega)e^{-j\omega t_0} \leftrightarrow x(t - t_0)$, (2.51) is converted to time-domain as

$$\hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, t) \approx (1 + \frac{\mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}{24c} (\frac{P_2}{c^2} - \Delta t^2) \frac{\partial^3}{\partial t^3}) \hat{\mathbf{E}}^{ref}(t_D) \quad (2.52)$$

where $t_D = t - \frac{\mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}{c}$. In the above expression, the $(j\omega)^3$ part is converted into a time-domain operator $\frac{\partial^3}{\partial t^3}$ that compensates the FDTD dispersion. It can be used to compute the incident fields at the TF/SF boundary with reduced errors. Note that this expression can be computed at every time step (on-the-fly) and thus the fields need not be determined and stored prior to the FDTD simulation.

The method in [91] requires lesser memory storage ($O(N^2)$) compared to the frequency-domain AFP method. However, since it approximates for FDTD dispersion and does not include frequency-dependent polarizations, the level of accuracy is much lower compared to the AFP method. The field leakage errors are about -40 dB, which is much higher than the -180 dB achieved by the AFP method.

In [92], an alternative approach was presented to compensate for FDTD dispersion in time-domain. This approach was presented for a focused light beam excitation, but it can be used for a plane wave excitation as well. In [92], the FDTD dispersion effect is compensated by correcting the phase velocity at the centre frequency of the source and for a given propagation direction. Since this method is a single-frequency compensation it may not be accurate for broadband source excitations. In addition, the method does not account for the non-orthogonality between the frequency-dependent field polarizations and the wavevector.

The TF/SF formulation has also been implemented in the implicit ADI-FDTD [95], [96] and LOD-FDTD [97] methods. Much similar to the TF/SF formulation for Yee's FDTD method, correction terms are deduced and applied to the ADI-FDTD and LOD-FDTD field update equations at the TF/SF boundary. The efforts in [95]-[97] do not however discuss the proper calculation of incident fields based on propagation in the implicit FDTD grids, as was discussed for the case of Yee's FDTD method.

2.5 Concluding Remarks

This chapter has reviewed several FDTD methods, namely, the explicit Yee's FDTD method as well as the implicit ADI and split-step FDTD methods. For each of these

FDTD methods, a summary of extensions to model anisotropic media along with the TF/SF formulation has been provided. From this literature survey, the following parts have been identified for further development, of which, the first two are related to extension of implicit FDTD methods for anisotropic media and the third is related to improving the accuracy of the time-domain analytic method in the Yee's FDTD TF/SF formulation:

We have identified a lack of implicit FDTD methods for treating 3-D wave propagation in general anisotropic media. The existing implicit FDTD methods have been generally developed for analysis of either 1-D wave propagation in anisotropic media characterized by 2-D constitutive tensors or 3-D wave propagation in anisotropic media characterized by diagonal constitutive tensors. The development of an implicit FDTD scheme for 3-D wave propagation in general anisotropic media is a challenging one as the method should firstly be stable and accurate even for time steps larger than the Courant-limit. Secondly, the method preferably should operate with efficient tridiagonal matrix solutions just as in the conventional ADI-FDTD and split-step FDTD methods. In Chapter 3, we present a novel implicit split-step FDTD method for 3-D wave propagation in general anisotropic media. The proposed method is verified to be stable and accurate even for time steps larger than the Courant-limit. Furthermore, the proposed method involves six tridiagonal matrix solutions, which is computationally equivalent to that required in the conventional split-step FDTD and ADI-FDTD methods.

In addition, we have noted that the existing complex-envelope (CE) ADI-FDTD method for analyzing anisotropic photonic crystals is unable to accomodate magnetic materials such as ferrite or gain materials. Periodic structures with such magnetic materials can support unique electromagnetic effects such as unidirectional wave propagation with vanishing group velocity and growth in wave amplitude. Periodic structures such as

cholesteric liquid crystals doped with laser dye can support circularly polarized lasing. In Chapter 4, we present an extension of the CE-ADI-FDTD method for anisotropic periodic structures composed of ferrite and gain media. This extension is formulated based on the fundamental ADI-FDTD splitting formulae. For nonmagnetic periodic structures, we show that the proposed method can reduce to a more efficient form compared to the conventional CE-ADI-FDTD method.

We have also identified that the time-domain analytic methods in the Yee's FDTD TF/SF formulation produce high field leakage errors of about -40 dB, compared to the frequency-domain analytic methods and the 1-D MAP grid method. Since time-domain analytic methods are useful in exciting both plane and non-plane waves and they require lesser memory storage, it would be beneficial to improve its level of accuracy. In Chapter 5, we present an accurate time-domain analytic method for computing incident fields in the Yee's FDTD TF/SF formulation. We demonstrate the level of accuracy achieved by considering both plane wave and focused beam excitations. Additional formulations are presented as well to facilitate the implementation of the proposed method.

Chapter 3

Split-Step FDTD Method for General Anisotropic Media

3.1 Introduction

In Section 2.3, several unconditionally stable implicit FDTD methods for anisotropic media were reviewed. These implicit FDTD methods are generally developed for the analysis of 1-D wave propagation in anisotropic media characterized by 2-D constitutive tensors as well as 3-D wave propagation in anisotropic media characterized by diagonal constitutive tensors. Despite these efforts, one of the existing challenges lies in the development of implicit FDTD methods for the analysis of 3-D wave propagation in general anisotropic media.

In this chapter, we present a novel implicit FDTD method based on the split-step scheme for 3-D Maxwell's equations in general anisotropic media. The general anisotropic media can be characterized by full permittivity and permeability tensors. Stability anal-

ysis of the proposed method in general anisotropic media is performed using the Fourier method. The eigenvalues of the Fourier amplification matrix are numerically shown to have unity magnitude even for time steps greater than the Courant-limit time step. This illustrates the stable and non-dissipative nature of the proposed split-step FDTD method in general anisotropic media. Extensions of the proposed split-step FDTD method with perfectly matched layer (PML) boundary conditions are presented as well, specifically for a TM_z problem. The formulation of this extension is presented in terms of the fundamental SS1 (split-step with first-order temporal accuracy) splitting formulae [26], that can result in update equations with fewer and simpler right-hand side (RHS) terms. Numerical examples from five different experiments are presented to validate the efficiency of the proposed method in general anisotropic media. This includes an example of a 2-D photonic crystal cavity infiltrated with anisotropic material to tune its resonant frequency.

The formulation of the proposed split-step FDTD method is first presented in Section 3.2. In that section, the original approach that was used to attain the formulation is first highlighted. Subsequently, a more formal approach is presented, from which we exemplify an extension of the split-step FDTD method to include PML boundary conditions. Section 3.3 next presents a stability analysis of the proposed split-step FDTD method using the Fourier method. Numerical results from five different experiments are then presented in Section 3.4 to validate the stability, accuracy and efficiency of the proposed split-step FDTD method in general anisotropic media. Section 3.5 finally provides the conclusion.

3.2 Formulation

In this section, we present the formulation of the proposed split-step FDTD method for 3-D Maxwell's equations in general anisotropic media, characterized by full permittivity ($\bar{\epsilon}$) and permeability ($\bar{\mu}$) tensors. The original approach from which the formulation was attained is presented first. Following which, a more formal approach is presented. This approach can be used to extend the split-step FDTD method to include for example PML boundary conditions, as will be exemplified in the final subsection.

3.2.1 Original Approach

For isotropic media, the split-step FDTD method is formulated as (2.15)-(2.16). Upon expansion of substep 1 in (2.15), equations of the following form can be derived for electric ($\mathbf{E}$) and magnetic ($\mathbf{H}$) field components :

$$E_z|^{n+\frac{1}{2}} = E_z|_n + \frac{\Delta t}{2\epsilon} \frac{\partial H_y|^{n+\frac{1}{2}}}{\partial x} + \frac{\Delta t}{2\epsilon} \frac{\partial H_y|_n}{\partial x} \quad (3.1)$$

$$H_y|^{n+\frac{1}{2}} = H_y|_n + \frac{\Delta t}{2\mu} \frac{\partial E_z|^{n+\frac{1}{2}}}{\partial x} + \frac{\Delta t}{2\mu} \frac{\partial E_z|_n}{\partial x}. \quad (3.2)$$

Update equations (3.1)-(3.2) for E_z and H_y field components form a pair of 1-D equations that can be efficiently solved via a linear system of equations with tridiagonal coefficient matrix. Three pairs of such 1-D equations are solved each in substeps 1 and 2.

For anisotropic media, the proposed split-step FDTD method splits the update of electric ($\mathbf{D}$) and magnetic ($\mathbf{B}$) flux components (instead of $\mathbf{E}$ and $\mathbf{H}$ field components as in isotropic media) over 6 substeps. Each substep involves a single pair of 1-D update equations with similar RHS as those for isotropic media. These 6 substeps are written

as

Substep 1

$$D_x|^{n,1} = D_x|^n, \quad B_x|^{n,1} = B_x|^n, \quad D_y|^{n,1} = D_y|^n, \quad B_z|^{n,1} = B_z|^n \quad (3.3)$$

$$D_z|^{n,1} = D_z|^n + \frac{\Delta t}{2} \frac{\partial H_y|^{n,1}}{\partial x} + \frac{\Delta t}{2} \frac{\partial H_y|^n}{\partial x} \quad (3.4)$$

$$B_y|^{n,1} = B_y|^n + \frac{\Delta t}{2} \frac{\partial E_z|^{n,1}}{\partial x} + \frac{\Delta t}{2} \frac{\partial E_z|^n}{\partial x} \quad (3.5)$$

Substep 2

$$D_y|^{n,2} = D_y|^{n,1}, \quad B_x|^{n,2} = B_x|^{n,1}, \quad D_z|^{n,2} = D_z|^{n,1}, \quad B_y|^{n,2} = B_y|^{n,1} \quad (3.6)$$

$$D_x|^{n,2} = D_x|^{n,1} + \frac{\Delta t}{2} \frac{\partial H_z|^{n,2}}{\partial y} + \frac{\Delta t}{2} \frac{\partial H_z|^{n,1}}{\partial y} \quad (3.7)$$

$$B_z|^{n,2} = B_z|^{n,1} + \frac{\Delta t}{2} \frac{\partial E_x|^{n,2}}{\partial y} + \frac{\Delta t}{2} \frac{\partial E_x|^{n,1}}{\partial y} \quad (3.8)$$

Substep 3

$$D_x|^{n,3} = D_x|^{n,2}, \quad B_y|^{n,3} = B_y|^{n,2}, \quad D_z|^{n,3} = D_z|^{n,2}, \quad B_z|^{n,3} = B_z|^{n,2} \quad (3.9)$$

$$D_y|^{n,3} = D_y|^{n,2} + \frac{\Delta t}{2} \frac{\partial H_x|^{n,3}}{\partial z} + \frac{\Delta t}{2} \frac{\partial H_x|^{n,2}}{\partial z} \quad (3.10)$$

$$B_x|^{n,3} = B_x|^{n,2} + \frac{\Delta t}{2} \frac{\partial E_y|^{n,3}}{\partial z} + \frac{\Delta t}{2} \frac{\partial E_y|^{n,2}}{\partial z} \quad (3.11)$$

Substep 4

$$D_x|^{n,4} = D_x|^{n,3}, \quad B_x|^{n,4} = B_x|^{n,3}, \quad D_z|^{n,4} = D_z|^{n,3}, \quad B_y|^{n,4} = B_y|^{n,3} \quad (3.12)$$

$$D_y|^{n,4} = D_y|^{n,3} - \frac{\Delta t}{2} \frac{\partial H_z|^{n,4}}{\partial x} - \frac{\Delta t}{2} \frac{\partial H_z|^{n,3}}{\partial x} \quad (3.13)$$

$$B_z|^{n,4} = B_z|^{n,3} - \frac{\Delta t}{2} \frac{\partial E_y|^{n,4}}{\partial x} - \frac{\Delta t}{2} \frac{\partial E_y|^{n,3}}{\partial x} \quad (3.14)$$

Substep 5

$$D_x|^{n,5} = D_x|^{n,4}, \quad B_y|^{n,5} = B_y|^{n,4}, \quad D_y|^{n,5} = D_y|^{n,4}, \quad B_z|^{n,5} = B_z|^{n,4} \quad (3.15)$$

$$D_z|^{n,5} = D_z|^{n,4} - \frac{\Delta t}{2} \frac{\partial H_x|^{n,5}}{\partial y} - \frac{\Delta t}{2} \frac{\partial H_x|^{n,4}}{\partial y} \quad (3.16)$$

$$B_x|^{n,5} = B_x|^{n,4} - \frac{\Delta t}{2} \frac{\partial E_z|^{n,5}}{\partial y} - \frac{\Delta t}{2} \frac{\partial E_z|^{n,4}}{\partial y} \quad (3.17)$$

Substep 6

$$D_y|^{n+1} = D_y|^{n,5}, \quad B_x|^{n+1} = B_x|^{n,5}, \quad D_z|^{n+1} = D_z|^{n,5}, \quad B_z|^{n+1} = B_z|^{n,5} \quad (3.18)$$

$$D_x|^{n+1} = D_x|^{n,5} - \frac{\Delta t}{2} \frac{\partial H_y|^{n+1}}{\partial z} - \frac{\Delta t}{2} \frac{\partial H_y|^{n,5}}{\partial z} \quad (3.19)$$

$$B_y|^{n+1} = B_y|^{n,5} - \frac{\Delta t}{2} \frac{\partial E_x|^{n+1}}{\partial z} - \frac{\Delta t}{2} \frac{\partial E_x|^{n,5}}{\partial z}. \quad (3.20)$$

By applying the inverse constitutive relations

$$\mathbf{E} = \bar{\bar{\mathbf{K}}}\mathbf{D}, \quad \bar{\bar{\mathbf{K}}} = \bar{\bar{\boldsymbol{\epsilon}}}^{-1} \quad (3.21)$$

$$\mathbf{H} = \bar{\bar{\mathbf{V}}}\mathbf{B}, \quad \bar{\bar{\mathbf{V}}} = \bar{\bar{\boldsymbol{\mu}}}^{-1} \quad (3.22)$$

to each substep and after some manipulations, the split-step FDTD method for 3-D Maxwell's equations in general anisotropic media, can be written in terms of only $\mathbf{E}$ - $\mathbf{H}$

field components as

Substep 1

$$E_z|^{n,1} = E_z|^n + \frac{\kappa_{zz}\Delta t}{2} \frac{\partial H_y|^{n,1}}{\partial x} + \frac{\kappa_{zz}\Delta t}{2} \frac{\partial H_y|^n}{\partial x} \quad (3.23)$$

$$H_y|^{n,1} = H_y|^n + \frac{v_{yy}\Delta t}{2} \frac{\partial E_z|^{n,1}}{\partial x} + \frac{v_{yy}\Delta t}{2} \frac{\partial E_z|^n}{\partial x} \quad (3.24)$$

$$E_x|^{n,1} = \frac{\kappa_{xz}}{\kappa_{zz}}(E_z|^{n,1} - E_z|^n) + E_x|^n \quad (3.25)$$

$$E_y|^{n,1} = \frac{\kappa_{yz}}{\kappa_{zz}}(E_z|^{n,1} - E_z|^n) + E_y|^n \quad (3.26)$$

$$H_x|^{n,1} = \frac{v_{xy}}{v_{yy}}(H_y|^{n,1} - H_y|^n) + H_x|^n \quad (3.27)$$

$$H_z|^{n,1} = \frac{v_{zy}}{v_{yy}}(H_y|^{n,1} - H_y|^n) + H_z|^n \quad (3.28)$$

Substep 2

$$E_x|^{n,2} = E_x|^{n,1} + \frac{\kappa_{xx}\Delta t}{2} \frac{\partial H_z|^{n,2}}{\partial y} + \frac{\kappa_{xx}\Delta t}{2} \frac{\partial H_z|^{n,1}}{\partial y} \quad (3.29)$$

$$H_z|^{n,2} = H_z|^{n,1} + \frac{v_{zz}\Delta t}{2} \frac{\partial E_x|^{n,2}}{\partial y} + \frac{v_{zz}\Delta t}{2} \frac{\partial E_x|^{n,1}}{\partial y} \quad (3.30)$$

$$E_y|^{n,2} = \frac{\kappa_{yx}}{\kappa_{xx}}(E_x|^{n,2} - E_x|^{n,1}) + E_y|^{n,1} \quad (3.31)$$

$$E_z|^{n,2} = \frac{\kappa_{zx}}{\kappa_{xx}}(E_x|^{n,2} - E_x|^{n,1}) + E_z|^{n,1} \quad (3.32)$$

$$H_x|^{n,2} = \frac{v_{xz}}{v_{zz}}(H_z|^{n,2} - H_z|^{n,1}) + H_x|^{n,1} \quad (3.33)$$

$$H_y|^{n,2} = \frac{v_{yz}}{v_{zz}}(H_z|^{n,2} - H_z|^{n,1}) + H_y|^{n,1} \quad (3.34)$$

Substep 3

$$E_y|^{n,3} = E_y|^{n,2} + \frac{\kappa_{yy}\Delta t}{2} \frac{\partial H_x|^{n,3}}{\partial z} + \frac{\kappa_{yy}\Delta t}{2} \frac{\partial H_x|^{n,2}}{\partial z} \quad (3.35)$$

$$H_x|^{n,3} = H_x|^{n,2} + \frac{\nu_{xx}\Delta t}{2} \frac{\partial E_y|^{n,3}}{\partial z} + \frac{\nu_{xx}\Delta t}{2} \frac{\partial E_y|^{n,2}}{\partial z} \quad (3.36)$$

$$E_x|^{n,3} = \frac{\kappa_{xy}}{\kappa_{yy}}(E_y|^{n,3} - E_y|^{n,2}) + E_x|^{n,2} \quad (3.37)$$

$$E_z|^{n,3} = \frac{\kappa_{zy}}{\kappa_{yy}}(E_y|^{n,3} - E_y|^{n,2}) + E_z|^{n,2} \quad (3.38)$$

$$H_y|^{n,3} = \frac{\nu_{yx}}{\nu_{xx}}(H_x|^{n,3} - H_x|^{n,2}) + H_y|^{n,2} \quad (3.39)$$

$$H_z|^{n,3} = \frac{\nu_{zx}}{\nu_{xx}}(H_x|^{n,3} - H_x|^{n,2}) + H_z|^{n,2} \quad (3.40)$$

Substep 4

$$E_y|^{n,4} = E_y|^{n,3} - \frac{\kappa_{yy}\Delta t}{2} \frac{\partial H_z|^{n,4}}{\partial x} - \frac{\kappa_{yy}\Delta t}{2} \frac{\partial H_z|^{n,3}}{\partial x} \quad (3.41)$$

$$H_z|^{n,4} = H_z|^{n,3} - \frac{\nu_{zz}\Delta t}{2} \frac{\partial E_y|^{n,4}}{\partial x} - \frac{\nu_{zz}\Delta t}{2} \frac{\partial E_y|^{n,3}}{\partial x} \quad (3.42)$$

$$E_x|^{n,4} = \frac{\kappa_{xy}}{\kappa_{yy}}(E_y|^{n,4} - E_y|^{n,3}) + E_x|^{n,3} \quad (3.43)$$

$$E_z|^{n,4} = \frac{\kappa_{zy}}{\kappa_{yy}}(E_y|^{n,4} - E_y|^{n,3}) + E_z|^{n,3} \quad (3.44)$$

$$H_x|^{n,4} = \frac{\nu_{xz}}{\nu_{zz}}(H_z|^{n,4} - H_z|^{n,3}) + H_x|^{n,3} \quad (3.45)$$

$$H_y|^{n,4} = \frac{\nu_{yz}}{\nu_{zz}}(H_z|^{n,4} - H_z|^{n,3}) + H_y|^{n,3} \quad (3.46)$$

Substep 5

$$E_z|^{n,5} = E_z|^{n,4} - \frac{\kappa_{zz}\Delta t}{2} \frac{\partial H_x|^{n,5}}{\partial y} - \frac{\kappa_{zz}\Delta t}{2} \frac{\partial H_x|^{n,4}}{\partial y} \quad (3.47)$$

$$H_x|^{n,5} = H_x|^{n,4} - \frac{\nu_{xx}\Delta t}{2} \frac{\partial E_z|^{n,5}}{\partial y} - \frac{\nu_{xx}\Delta t}{2} \frac{\partial E_z|^{n,4}}{\partial y} \quad (3.48)$$

$$E_x|^{n,5} = \frac{\kappa_{xz}}{\kappa_{zz}}(E_z|^{n,5} - E_z|^{n,4}) + E_x|^{n,4} \quad (3.49)$$

$$E_y|^{n,5} = \frac{\kappa_{yz}}{\kappa_{zz}}(E_z|^{n,5} - E_z|^{n,4}) + E_y|^{n,4} \quad (3.50)$$

$$H_y|^{n,5} = \frac{\nu_{yx}}{\nu_{xx}}(H_x|^{n,5} - H_x|^{n,4}) + H_y|^{n,4} \quad (3.51)$$

$$H_z|^{n,5} = \frac{\nu_{zx}}{\nu_{xx}}(H_x|^{n,5} - H_x|^{n,4}) + H_z|^{n,4} \quad (3.52)$$

Substep 6

$$E_x|^{n+1} = E_x|^{n,5} - \frac{\kappa_{xx}\Delta t}{2} \frac{\partial H_y|^{n+1}}{\partial z} - \frac{\kappa_{xx}\Delta t}{2} \frac{\partial H_y|^{n,5}}{\partial z} \quad (3.53)$$

$$H_y|^{n+1} = H_y|^{n,5} - \frac{\nu_{yy}\Delta t}{2} \frac{\partial E_x|^{n+1}}{\partial z} - \frac{\nu_{yy}\Delta t}{2} \frac{\partial E_x|^{n,5}}{\partial z} \quad (3.54)$$

$$E_y|^{n+1} = \frac{\kappa_{yx}}{\kappa_{xx}}(E_x|^{n+1} - E_x|^{n,5}) + E_y|^{n,5} \quad (3.55)$$

$$E_z|^{n+1} = \frac{\kappa_{zx}}{\kappa_{xx}}(E_x|^{n+1} - E_x|^{n,5}) + E_z|^{n,5} \quad (3.56)$$

$$H_x|^{n+1} = \frac{\nu_{xy}}{\nu_{yy}}(H_y|^{n+1} - H_y|^{n,5}) + H_x|^{n,5} \quad (3.57)$$

$$H_z|^{n+1} = \frac{\nu_{zy}}{\nu_{yy}}(H_y|^{n+1} - H_y|^{n,5}) + H_z|^{n,5}. \quad (3.58)$$

Note firstly that when $\bar{\bar{\epsilon}}$ and $\bar{\bar{\mu}}$ are isotropic or diagonal, the formulation Substep 1 to Substep 6 reduces to the conventional split-step FDTD method as presented in (2.15)-(2.16). Secondly, apart from the 4 explicit equations in each substep, such as (3.25)-(3.28) in Substep 1, the entire update from n to $n+1$ requires the solution of 6 pairs of implicit 1-D equations. This requirement is the same as the conventional split-step FDTD method, where the solutions of 6 pairs of implicit 1-D equations are achieved over 2 substeps (three in each substep). Thirdly, in every substep, the fields in the implicit

1-D equations are determined via efficient tridiagonal matrix solutions.

Next, we discuss the actual numerical update of the electric and magnetic field components. For spatial discretization, we assume the use of Yee's grid. Consider Substep 1 as an illustration. By substituting the RHS of (3.24) into (3.23) and after some manipulations, the implicit update of $E_z|_{i,j,k+\frac{1}{2}}^{n,1}$ is performed as

$$\begin{aligned} & -\frac{\Delta t^2 \kappa_{zz} \nu_{yy}}{4\Delta x^2} E_z|_{i-1,j,k+\frac{1}{2}}^{n,1} + \left(1 + \frac{\Delta t^2 \kappa_{zz} \nu_{yy}}{2\Delta x^2}\right) E_z|_{i,j,k+\frac{1}{2}}^{n,1} - \frac{\Delta t^2 \kappa_{zz} \nu_{yy}}{4\Delta x^2} E_z|_{i+1,j,k+\frac{1}{2}}^{n,1} \\ & = E_z|_{i,j,k+\frac{1}{2}}^n + \frac{\Delta t \kappa_{zz}}{\Delta x} (H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n - H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^n) \\ & + \frac{\Delta t^2 \kappa_{zz} \nu_{yy}}{4\Delta x^2} (E_z|_{i-1,j,k+\frac{1}{2}}^n - 2E_z|_{i,j,k+\frac{1}{2}}^n + E_z|_{i+1,j,k+\frac{1}{2}}^n). \end{aligned} \quad (3.59)$$

With (3.59), a system of linear equations with tridiagonal coefficient matrix is formed and the update of $E_z|_{i,j,k+\frac{1}{2}}^{n,1}$ is efficiently carried out. Subsequently the update of $H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n,1}$ is determined as

$$\begin{aligned} H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n,1} & = H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n + \frac{\Delta t \nu_{yy}}{2\Delta x} (E_z|_{i+1,j,k+\frac{1}{2}}^{n,1} - E_z|_{i,j,k+\frac{1}{2}}^{n,1}) \\ & + \frac{\Delta t \nu_{yy}}{2\Delta x} (E_z|_{i+1,j,k+\frac{1}{2}}^n - E_z|_{i,j,k+\frac{1}{2}}^n). \end{aligned} \quad (3.60)$$

Upon updating $E_z|_{i,j,k+\frac{1}{2}}^{n,1}$ and $H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n,1}$, the updates of remaining field components are performed using the 4 explicit update equations (3.25)-(3.28). Note that at every field point on the Yee's grid, only one field component is directly available. The remaining field components that are not directly available are attained by interpolation from four values in the neighboring grid points. Such interpolations are performed in (3.25)-(3.28). As an example, in the update of $E_x|_{i+\frac{1}{2},j,k}^{n,1}$ in (3.25), the value of $E_z|_{i+\frac{1}{2},j,k}^{n,1}$

is attained by

$$E_z|_{i+\frac{1}{2},j,k}^{n,1} = \frac{1}{4}(E_z|_{i,j,k+\frac{1}{2}}^{n,1} + E_z|_{i+1,j,k+\frac{1}{2}}^{n,1} + E_z|_{i,j,k-\frac{1}{2}}^{n,1} + E_z|_{i+1,j,k-\frac{1}{2}}^{n,1}). \quad (3.61)$$

Similar type of interpolations were performed in [28]. The updates of electric and magnetic field components in Substep 2 to Substep 6 are performed in a similar manner discussed above.

3.2.2 Formal Matrix Approach

In this section, an alternative and formal approach to derive the proposed split-step FDTD method is presented. The 3-D Maxwell's equations that describe electromagnetic wave propagation in a sourceless anisotropic media is

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} \quad (3.62)$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}. \quad (3.63)$$

Applying the inverse constitutive relations $\mathbf{E} = \bar{\bar{\mathbf{K}}}\mathbf{D}$ and $\mathbf{H} = \bar{\bar{\mathbf{V}}}\mathbf{B}$ in (3.62)-(3.63) gives

$$\frac{\partial \mathbf{E}}{\partial t} = \bar{\bar{\mathbf{K}}}\nabla \times \mathbf{H} \quad (3.64)$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\bar{\bar{\mathbf{V}}}\nabla \times \mathbf{E}. \quad (3.65)$$

Maxwell's equations (3.64)-(3.65) can be expressed as a first-order differential system

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{M}\mathbf{u}, \quad (3.66)$$

where

$$\mathbf{u} = \begin{bmatrix} E_x & E_y & E_z & H_x & H_y & H_z \end{bmatrix}^T \quad (3.67)$$

and

$$\mathbf{M} = \begin{bmatrix} \mathbf{0} & \mathbf{M}_K \\ \mathbf{M}_V & \mathbf{0} \end{bmatrix} \quad (3.68)$$

with

$$\mathbf{M}_K = \begin{bmatrix} \kappa_{xy} \frac{\partial}{\partial z} - \kappa_{xz} \frac{\partial}{\partial y} & -\kappa_{xx} \frac{\partial}{\partial z} + \kappa_{xz} \frac{\partial}{\partial x} & \kappa_{xx} \frac{\partial}{\partial y} - \kappa_{xy} \frac{\partial}{\partial x} \\ \kappa_{yy} \frac{\partial}{\partial z} - \kappa_{yz} \frac{\partial}{\partial y} & -\kappa_{yx} \frac{\partial}{\partial z} + \kappa_{yz} \frac{\partial}{\partial x} & \kappa_{yx} \frac{\partial}{\partial y} - \kappa_{yy} \frac{\partial}{\partial x} \\ \kappa_{zy} \frac{\partial}{\partial z} - \kappa_{zz} \frac{\partial}{\partial y} & -\kappa_{zx} \frac{\partial}{\partial z} + \kappa_{zz} \frac{\partial}{\partial x} & \kappa_{zx} \frac{\partial}{\partial y} - \kappa_{zy} \frac{\partial}{\partial x} \end{bmatrix},$$

$$\mathbf{M}_V = \begin{bmatrix} -v_{xy} \frac{\partial}{\partial z} + v_{xz} \frac{\partial}{\partial y} & v_{xx} \frac{\partial}{\partial z} - v_{xz} \frac{\partial}{\partial x} & -v_{xx} \frac{\partial}{\partial y} + v_{xy} \frac{\partial}{\partial x} \\ -v_{yy} \frac{\partial}{\partial z} + v_{yz} \frac{\partial}{\partial y} & v_{yx} \frac{\partial}{\partial z} - v_{yz} \frac{\partial}{\partial x} & -v_{yx} \frac{\partial}{\partial y} + v_{yy} \frac{\partial}{\partial x} \\ -v_{zy} \frac{\partial}{\partial z} + v_{zz} \frac{\partial}{\partial y} & v_{zx} \frac{\partial}{\partial z} - v_{zz} \frac{\partial}{\partial x} & -v_{zx} \frac{\partial}{\partial y} + v_{zy} \frac{\partial}{\partial x} \end{bmatrix}$$

and $\mathbf{0}$ is the null matrix. Matrix $\mathbf{M}$ includes spatial derivative operators associated with corresponding elements of the inverse permittivity ($\bar{\bar{\kappa}}$) and permeability ($\bar{\bar{v}}$) tensors.

The solution of (3.66) is expressed as

$$\mathbf{u}(t) = e^{\mathbf{M}t} \mathbf{u}(t_0), \quad (3.69)$$

where $e^{\mathbf{M}t}$ is the matrix exponential operator and $\mathbf{u}(t_0)$ is the initial state of the system at time t_0 . An update equation of (3.69) from n to $n+1$ can be attained as

$$\mathbf{u}^{n+1} = e^{\mathbf{M}\Delta t} \mathbf{u}^n. \quad (3.70)$$

The proposed split-step FDTD method can now be attained by first splitting the matrix exponential operator $e^{\mathbf{M}\Delta t}$ correct to first-order as

$$e^{\mathbf{M}\Delta t} \approx e^{\mathbf{F}\Delta t} e^{\mathbf{E}\Delta t} e^{\mathbf{D}\Delta t} e^{\mathbf{C}\Delta t} e^{\mathbf{B}\Delta t} e^{\mathbf{A}\Delta t}, \quad (3.71)$$

in which matrix $\mathbf{M} = \mathbf{A} + \mathbf{B} + \mathbf{C} + \mathbf{D} + \mathbf{E} + \mathbf{F}$. Matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$, $\mathbf{E}$ and $\mathbf{F}$ contain only the $+\frac{\partial}{\partial x}$, $+\frac{\partial}{\partial y}$, $+\frac{\partial}{\partial z}$, $-\frac{\partial}{\partial x}$, $-\frac{\partial}{\partial y}$ and $-\frac{\partial}{\partial z}$ operators, respectively, as

$$\begin{aligned} \mathbf{A} &= \begin{bmatrix} 0 & 0 & 0 & 0 & \kappa_{xz} \frac{\partial}{\partial x} & 0 \\ 0 & 0 & 0 & 0 & \kappa_{yz} \frac{\partial}{\partial x} & 0 \\ 0 & 0 & 0 & 0 & \kappa_{zz} \frac{\partial}{\partial x} & 0 \\ 0 & 0 & v_{xy} \frac{\partial}{\partial x} & 0 & 0 & 0 \\ 0 & 0 & v_{yy} \frac{\partial}{\partial x} & 0 & 0 & 0 \\ 0 & 0 & v_{zy} \frac{\partial}{\partial x} & 0 & 0 & 0 \end{bmatrix} & \mathbf{B} &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \kappa_{xx} \frac{\partial}{\partial y} \\ 0 & 0 & 0 & 0 & 0 & \kappa_{yx} \frac{\partial}{\partial y} \\ 0 & 0 & 0 & 0 & 0 & \kappa_{zx} \frac{\partial}{\partial y} \\ v_{xz} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 & 0 \\ v_{yz} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 & 0 \\ v_{zz} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \\ \mathbf{C} &= \begin{bmatrix} 0 & 0 & 0 & \kappa_{xy} \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 & \kappa_{yy} \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 & \kappa_{zy} \frac{\partial}{\partial z} & 0 & 0 \\ 0 & v_{xx} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \\ 0 & v_{yx} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \\ 0 & v_{zx} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \end{bmatrix} & \mathbf{D} &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\kappa_{xy} \frac{\partial}{\partial x} \\ 0 & 0 & 0 & 0 & 0 & -\kappa_{yy} \frac{\partial}{\partial x} \\ 0 & 0 & 0 & 0 & 0 & -\kappa_{zy} \frac{\partial}{\partial x} \\ 0 & -v_{xz} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ 0 & -v_{yz} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ 0 & -v_{zz} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \end{bmatrix} \\ \mathbf{E} &= \begin{bmatrix} 0 & 0 & 0 & -\kappa_{xz} \frac{\partial}{\partial y} & 0 & 0 \\ 0 & 0 & 0 & -\kappa_{yz} \frac{\partial}{\partial y} & 0 & 0 \\ 0 & 0 & 0 & -\kappa_{zz} \frac{\partial}{\partial y} & 0 & 0 \\ 0 & 0 & -v_{xx} \frac{\partial}{\partial y} & 0 & 0 & 0 \\ 0 & 0 & -v_{yx} \frac{\partial}{\partial y} & 0 & 0 & 0 \\ 0 & 0 & -v_{zx} \frac{\partial}{\partial y} & 0 & 0 & 0 \end{bmatrix} & \mathbf{F} &= \begin{bmatrix} 0 & 0 & 0 & 0 & -\kappa_{xx} \frac{\partial}{\partial z} & 0 \\ 0 & 0 & 0 & 0 & -\kappa_{yx} \frac{\partial}{\partial z} & 0 \\ 0 & 0 & 0 & 0 & -\kappa_{zx} \frac{\partial}{\partial z} & 0 \\ -v_{xy} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \\ -v_{yy} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \\ -v_{zy} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \end{aligned}$$

Next, by substituting (3.71) into (3.70) and splitting the entire update of n to $n + 1$ into 6 substeps, the following set of update equations is attained

$$\begin{aligned}
\mathbf{u}^{n,1} &= e^{\mathbf{A}\Delta t} \mathbf{u}^n \\
\mathbf{u}^{n,2} &= e^{\mathbf{B}\Delta t} \mathbf{u}^{n,1} \\
\mathbf{u}^{n,3} &= e^{\mathbf{C}\Delta t} \mathbf{u}^{n,2} \\
\mathbf{u}^{n,4} &= e^{\mathbf{D}\Delta t} \mathbf{u}^{n,3} \\
\mathbf{u}^{n,5} &= e^{\mathbf{E}\Delta t} \mathbf{u}^{n,4} \\
\mathbf{u}^{n+1} &= e^{\mathbf{F}\Delta t} \mathbf{u}^{n,5}.
\end{aligned} \tag{3.72}$$

Each matrix exponential operator in (3.72) is next replaced by a second-order approximation, for example, $e^{\mathbf{Z}} = (\mathbf{I} - \frac{1}{2}\mathbf{Z})^{-1}(\mathbf{I} + \frac{1}{2}\mathbf{Z})$ where $\mathbf{I}$ is the identity matrix. After left-multiplying every equation by $(\mathbf{I} - \frac{1}{2}\mathbf{Z})$, the proposed split-step FDTD method is finally arrived at in compact form as

$$\begin{aligned}
(\mathbf{I} - \frac{\Delta t}{2}\mathbf{A})\mathbf{u}^{n,1} &= (\mathbf{I} + \frac{\Delta t}{2}\mathbf{A})\mathbf{u}^n \\
(\mathbf{I} - \frac{\Delta t}{2}\mathbf{B})\mathbf{u}^{n,2} &= (\mathbf{I} + \frac{\Delta t}{2}\mathbf{B})\mathbf{u}^{n,1} \\
(\mathbf{I} - \frac{\Delta t}{2}\mathbf{C})\mathbf{u}^{n,3} &= (\mathbf{I} + \frac{\Delta t}{2}\mathbf{C})\mathbf{u}^{n,2} \\
(\mathbf{I} - \frac{\Delta t}{2}\mathbf{D})\mathbf{u}^{n,4} &= (\mathbf{I} + \frac{\Delta t}{2}\mathbf{D})\mathbf{u}^{n,3} \\
(\mathbf{I} - \frac{\Delta t}{2}\mathbf{E})\mathbf{u}^{n,5} &= (\mathbf{I} + \frac{\Delta t}{2}\mathbf{E})\mathbf{u}^{n,4} \\
(\mathbf{I} - \frac{\Delta t}{2}\mathbf{F})\mathbf{u}^{n+1} &= (\mathbf{I} + \frac{\Delta t}{2}\mathbf{F})\mathbf{u}^{n,5}.
\end{aligned} \tag{3.73}$$

Expanding this compact form results in the proposed split-step FDTD update equations in terms of $\mathbf{E}$ - $\mathbf{H}$ field components in Section 3.2.1.

3.2.3 An Extension with PML Boundary Conditions

In this section, we present an extension of the proposed split-step FDTD method with perfectly matched layer (PML) boundary conditions. The formulation is attained using the splitting approach presented in the previous subsection. The extension is presented for a 2-D TM_z problem with media characterized by scalar permittivity and tensor permeability.

Consider the following frequency-domain Maxwell's equations in anisotropic media:

$$j\omega\epsilon_0\tilde{\mathbf{E}} = \bar{\bar{\mathbf{k}}}_r\tilde{\nabla} \times \tilde{\mathbf{H}}, \quad (3.74)$$

$$j\omega\mu_0\tilde{\mathbf{H}} = -\bar{\bar{\mathbf{v}}}_r\tilde{\nabla} \times \tilde{\mathbf{E}}. \quad (3.75)$$

$\bar{\bar{\mathbf{k}}}_r$ and $\bar{\bar{\mathbf{v}}}_r$ represent the relative inverse permittivity and permeability tensors, respectively. $\tilde{\nabla}$ is the modified nabla operator that incorporates the complex-space version of the PML. $\tilde{\nabla}$ is given as

$$\tilde{\nabla} = \frac{1}{s_x} \frac{\partial}{\partial x} \hat{x} + \frac{1}{s_y} \frac{\partial}{\partial y} \hat{y} + \frac{1}{s_z} \frac{\partial}{\partial z} \hat{z}, \quad (3.76)$$

with coordinate-stretching variables $s_\xi = 1 + \frac{\sigma_\xi}{j\omega\epsilon_0}$ and PML conductivity σ_ξ along the direction $\xi = x, y, z$ [66]. In a split-field formulation, (3.74) can be decomposed as

$$j\omega\tilde{\mathbf{E}}_{s\xi}s_\xi = \frac{\bar{\bar{\mathbf{k}}}_r}{\epsilon_0} \frac{\partial}{\partial \xi} \hat{\xi} \times \tilde{\mathbf{H}}, \quad (3.77)$$

for $\xi = x, y, z$, with the original electric field vector $\tilde{\mathbf{E}}$ related to its split-field vectors $\tilde{\mathbf{E}}_{s\xi}$ as $\tilde{\mathbf{E}} = \tilde{\mathbf{E}}_{sx} + \tilde{\mathbf{E}}_{sy} + \tilde{\mathbf{E}}_{sz}$ [57]. A similar split-field formulation can be obtained for (3.75). Using the inverse Fourier transform, the corresponding time-domain split-field

equations can be attained as

$$\frac{\partial \mathbf{E}_{s\xi}}{\partial t} + \frac{\sigma_\xi}{\epsilon_0} \mathbf{E}_{s\xi} = \frac{\bar{\bar{\mathbf{k}}}_r}{\epsilon_0} \frac{\partial}{\partial \xi} \hat{\xi} \times \mathbf{H}, \quad (3.78)$$

$$\frac{\partial \mathbf{H}_{s\xi}}{\partial t} + \frac{\sigma_\xi}{\epsilon_0} \mathbf{H}_{s\xi} = -\frac{\bar{\bar{\mathbf{v}}}_r}{\mu_0} \frac{\partial}{\partial \xi} \hat{\xi} \times \mathbf{E}, \quad (3.79)$$

for $\xi = x, y, z$, with $\mathbf{E} = \mathbf{E}_{sx} + \mathbf{E}_{sy} + \mathbf{E}_{sz}$ and $\mathbf{H} = \mathbf{H}_{sx} + \mathbf{H}_{sy} + \mathbf{H}_{sz}$.

Considering a 2-D TM_z problem with scalar permittivity and tensor permeability (with elements $\mu_{xz} = \mu_{zx} = \mu_{yz} = \mu_{zy} = 0$), (3.78)-(3.79) reduce to six equations that can be expressed as a first-order differential system

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{M} \mathbf{u} \quad (3.80)$$

in which split-field vector $\mathbf{u}$ is

$$\mathbf{u} = \begin{bmatrix} E_{sx,z} & E_{sy,z} & H_{sx,x} & H_{sx,y} & H_{sy,x} & H_{sy,y} \end{bmatrix}^T \quad (3.81)$$

and matrix $\mathbf{M}$ is

$$\mathbf{M} = \begin{bmatrix} -\frac{\sigma_x}{\epsilon_0} & 0 & 0 & \frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial x} & 0 & \frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial x} \\ 0 & -\frac{\sigma_y}{\epsilon_0} & -\frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial y} & 0 & -\frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial y} & 0 \\ \frac{v_{xyr}}{\mu_0} \frac{\partial}{\partial x} & \frac{v_{xyr}}{\mu_0} \frac{\partial}{\partial x} & -\frac{\sigma_x}{\epsilon_0} & 0 & 0 & 0 \\ \frac{v_{yyr}}{\mu_0} \frac{\partial}{\partial x} & \frac{v_{yyr}}{\mu_0} \frac{\partial}{\partial x} & 0 & -\frac{\sigma_x}{\epsilon_0} & 0 & 0 \\ -\frac{v_{xxr}}{\mu_0} \frac{\partial}{\partial y} & -\frac{v_{xxr}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & -\frac{\sigma_y}{\epsilon_0} & 0 \\ -\frac{v_{yxr}}{\mu_0} \frac{\partial}{\partial y} & -\frac{v_{yxr}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & -\frac{\sigma_y}{\epsilon_0} \end{bmatrix}. \quad (3.82)$$

The original fields can be obtained from components of $\mathbf{u}$ as

$$\begin{aligned} E_z &= E_{sx,z} + E_{sy,z} \\ H_x &= H_{sx,x} + H_{sy,x} \\ H_y &= H_{sx,y} + H_{sy,y}. \end{aligned} \quad (3.83)$$

From (3.82), matrix $\mathbf{M}$ can be noted to contain only two types of spatial derivative operators, namely, $+\frac{\partial}{\partial x}$ and $-\frac{\partial}{\partial y}$.

Based on the splitting approach in Section 3.2.2, the split-step FDTD method for updating $\mathbf{u}$ can be written as

$$(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{A}) \mathbf{u}^n, \quad (3.84)$$

$$(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B}) \mathbf{u}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{B}) \mathbf{u}^{n+\frac{1}{2}}, \quad (3.85)$$

in which matrices $\mathbf{A}$ and $\mathbf{B}$ contain operators $+\frac{\partial}{\partial x}$ and $-\frac{\partial}{\partial y}$, respectively, as

$$\mathbf{A} = \begin{bmatrix} -\frac{\sigma_x}{2\epsilon_0} & 0 & 0 & \frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial x} & 0 & \frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial x} \\ 0 & -\frac{\sigma_y}{2\epsilon_0} & 0 & 0 & 0 & 0 \\ \frac{v_{xyr}}{\mu_0} \frac{\partial}{\partial x} & \frac{v_{xyr}}{\mu_0} \frac{\partial}{\partial x} & -\frac{\sigma_x}{2\epsilon_0} & 0 & 0 & 0 \\ \frac{v_{yyr}}{\mu_0} \frac{\partial}{\partial x} & \frac{v_{yyr}}{\mu_0} \frac{\partial}{\partial x} & 0 & -\frac{\sigma_x}{2\epsilon_0} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sigma_y}{2\epsilon_0} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sigma_y}{2\epsilon_0} \end{bmatrix} \quad (3.86)$$

$$\mathbf{B} = \begin{bmatrix} -\frac{\sigma_x}{2\epsilon_0} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sigma_y}{2\epsilon_0} & -\frac{1}{\epsilon_r\epsilon_0} \frac{\partial}{\partial y} & 0 & -\frac{1}{\epsilon_r\epsilon_0} \frac{\partial}{\partial y} & 0 \\ 0 & 0 & -\frac{\sigma_x}{2\epsilon_0} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sigma_x}{2\epsilon_0} & 0 & 0 \\ -\frac{v_{xxr}}{\mu_0} \frac{\partial}{\partial y} & -\frac{v_{xxr}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & -\frac{\sigma_y}{2\epsilon_0} & 0 \\ -\frac{v_{yxr}}{\mu_0} \frac{\partial}{\partial y} & -\frac{v_{yxr}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & -\frac{\sigma_y}{2\epsilon_0} \end{bmatrix}, \quad (3.87)$$

and matrix $\mathbf{M} = \mathbf{A} + \mathbf{B}$.

Since only two matrices are involved for this 2-D case, a more efficient form of (3.84)-(3.85) can readily be attained using the fundamental SS1 splitting formulae [26]. This efficient form can be written in compact form as

$$\text{Input initialization : } \hat{\mathbf{u}}^n = \mathbf{D}_{Diag}^{-1} \mathbf{u}^n, \quad (3.88)$$

$$\text{Substep 1 : } (\mathbf{I} - \frac{\Delta t}{4} \hat{\mathbf{A}}) \mathbf{v}^{n+\frac{1}{2}} = \hat{\mathbf{u}}^n, \quad (3.89)$$

$$\hat{\mathbf{u}}^{n+\frac{1}{2}} = \mathbf{D}_{Diag}^{-1} \mathbf{v}^{n+\frac{1}{2}} - \hat{\mathbf{u}}^n, \quad (3.90)$$

$$\text{Substep 2 : } (\mathbf{I} - \frac{\Delta t}{4} \hat{\mathbf{B}}) \mathbf{v}^{n+1} = \hat{\mathbf{u}}^{n+\frac{1}{2}}, \quad (3.91)$$

$$\hat{\mathbf{u}}^{n+1} = \mathbf{D}_{Diag}^{-1} \mathbf{v}^{n+1} - \hat{\mathbf{u}}^{n+\frac{1}{2}}, \quad (3.92)$$

$$\text{Output : } \mathbf{u}^{n+1} = \mathbf{D}_{Diag} \hat{\mathbf{u}}^{n+1}, \quad (3.93)$$

where $\mathbf{v}$ is an auxiliary vector denoted as

$$\mathbf{v} = \begin{bmatrix} e_{sx,z} & e_{sy,z} & h_{sx,x} & h_{sx,y} & h_{sy,x} & h_{sy,y} \end{bmatrix}^T \quad (3.94)$$

and matrices $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$ and diagonal matrix $\mathbf{D}_{Diag}$ are

$$\hat{\mathbf{A}} = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & 0 & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{v_{xyr}}{\mu_0} \frac{\partial}{\partial x} & \frac{v_{xyr}}{\mu_0} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \\ \frac{v_{yyr}}{\mu_0} \frac{\partial}{\partial x} & \frac{v_{yyr}}{\mu_0} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (3.95)$$

$$\hat{\mathbf{B}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial y} & 0 & -\frac{1}{\epsilon_r \epsilon_0} \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{v_{xxr}}{\mu_0} \frac{\partial}{\partial y} & -\frac{v_{xxr}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \\ -\frac{v_{yxr}}{\mu_0} \frac{\partial}{\partial y} & -\frac{v_{yxr}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 \\ \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0} & 0 & 0 & 0 & 0 \end{bmatrix} \quad (3.96)$$

$$\mathbf{D}_{Diag} = \text{diag}\left(\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}, \frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}\right). \quad (3.97)$$

Note that for zero initial fields, input initialization (3.88) need not be performed. In addition, the final fields can be output using (3.93), only when required. In the split-step formulation (3.89)-(3.92), the entire update from n to $n+1$ is split into two substeps, n to $n + \frac{1}{2}$ and $n + \frac{1}{2}$ to $n+1$. In each substep, the auxiliary fields are first updated using implicit/explicit update equations. The intermediate/final fields are subsequently updated using explicit equations only.

The compact form (3.88)-(3.93) can be expanded to give the following set of update equations:

Input initialization

$$\hat{E}_{sx,z}|^n = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} E_{sx,z}|^n, \quad \hat{E}_{sy,z}|^n = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} E_{sy,z}|^n \quad (3.98)$$

$$\hat{H}_{sx,x}|^n = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} H_{sx,x}|^n, \quad \hat{H}_{sx,y}|^n = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} H_{sx,y}|^n \quad (3.99)$$

$$\hat{H}_{sy,x}|^n = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} H_{sy,x}|^n, \quad \hat{H}_{sy,y}|^n = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} H_{sy,y}|^n \quad (3.100)$$

Substep 1

Auxiliary updating of $\mathbf{v}^{n+\frac{1}{2}}$ in (3.89):

$$e_{sx,z}|^{n+\frac{1}{2}} = \hat{E}_{sx,z}|^n + \frac{\frac{\Delta t}{4\epsilon_r \epsilon_0}}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} \left(\frac{\partial h_{sx,y}|^{n+\frac{1}{2}}}{\partial x} + \frac{\partial h_{sy,y}|^{n+\frac{1}{2}}}{\partial x} \right) \quad (3.101)$$

$$e_{sy,z}|^{n+\frac{1}{2}} = \hat{E}_{sy,z}|^n \quad (3.102)$$

$$h_{sx,x}|^{n+\frac{1}{2}} = \hat{H}_{sx,x}|^n + \frac{\frac{\Delta t v_{xyr}}{4\mu_0}}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} \left(\frac{\partial e_{sx,z}|^{n+\frac{1}{2}}}{\partial x} + \frac{\partial e_{sy,z}|^{n+\frac{1}{2}}}{\partial x} \right) \quad (3.103)$$

$$h_{sx,y}|^{n+\frac{1}{2}} = \hat{H}_{sx,y}|^n + \frac{\frac{\Delta t v_{yyr}}{4\mu_0}}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} \left(\frac{\partial e_{sx,z}|^{n+\frac{1}{2}}}{\partial x} + \frac{\partial e_{sy,z}|^{n+\frac{1}{2}}}{\partial x} \right) \quad (3.104)$$

$$h_{sy,x}|^{n+\frac{1}{2}} = \hat{H}_{sy,x}|^n \quad (3.105)$$

$$h_{sy,y}|^{n+\frac{1}{2}} = \hat{H}_{sy,y}|^n \quad (3.106)$$

Intermediate updating of $\hat{\mathbf{u}}^{n+\frac{1}{2}}$ in (3.90):

$$\hat{E}_{sx,z}|^{n+\frac{1}{2}} = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} e_{sx,z}|^{n+\frac{1}{2}} - \hat{E}_{sx,z}|^n \quad (3.107)$$

$$\hat{E}_{sy,z}|^{n+\frac{1}{2}} = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} e_{sy,z}|^{n+\frac{1}{2}} - \hat{E}_{sy,z}|^n \quad (3.108)$$

$$\hat{H}_{sx,x}|^{n+\frac{1}{2}} = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} h_{sx,x}|^{n+\frac{1}{2}} - \hat{H}_{sx,x}|^n \quad (3.109)$$

$$\hat{H}_{sx,y}|^{n+\frac{1}{2}} = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} h_{sx,y}|^{n+\frac{1}{2}} - \hat{H}_{sx,y}|^n \quad (3.110)$$

$$\hat{H}_{sy,x}|^{n+\frac{1}{2}} = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} h_{sy,x}|^{n+\frac{1}{2}} - \hat{H}_{sy,x}|^n \quad (3.111)$$

$$\hat{H}_{sy,y}|^{n+\frac{1}{2}} = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} h_{sy,y}|^{n+\frac{1}{2}} - \hat{H}_{sy,y}|^n \quad (3.112)$$

Substep 2

Auxiliary updating of $\mathbf{v}^{n+1}$ in (3.91):

$$e_{sx,z}|^{n+1} = \hat{E}_{sx,z}|^{n+\frac{1}{2}} \quad (3.113)$$

$$e_{sy,z}|^{n+1} = \hat{E}_{sy,z}|^{n+\frac{1}{2}} - \frac{\frac{\Delta t}{4\epsilon_r \epsilon_0}}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} \left(\frac{\partial h_{sx,x}|^{n+1}}{\partial y} + \frac{\partial h_{sy,x}|^{n+1}}{\partial y} \right) \quad (3.114)$$

$$h_{sx,x}|^{n+1} = \hat{H}_{sx,x}|^{n+\frac{1}{2}} \quad (3.115)$$

$$h_{sx,y}|^{n+1} = \hat{H}_{sx,y}|^{n+\frac{1}{2}} \quad (3.116)$$

$$h_{sy,x}|^{n+1} = \hat{H}_{sy,x}|^{n+\frac{1}{2}} - \frac{\frac{\Delta t v_{xxr}}{4\mu_0}}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} \left(\frac{\partial e_{sx,z}|^{n+1}}{\partial y} + \frac{\partial e_{sy,z}|^{n+1}}{\partial y} \right) \quad (3.117)$$

$$h_{sy,y}|^{n+1} = \hat{H}_{sy,y}|^{n+\frac{1}{2}} - \frac{\frac{\Delta t v_{yxr}}{4\mu_0}}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} \left(\frac{\partial e_{sx,z}|^{n+1}}{\partial y} + \frac{\partial e_{sy,z}|^{n+1}}{\partial y} \right) \quad (3.118)$$

Final updating of $\hat{\mathbf{u}}^{n+1}$ in (3.92):

$$\hat{E}_{sx,z}|^{n+1} = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} e_{sx,z}|^{n+1} - \hat{E}_{sx,z}|^{n+\frac{1}{2}} \quad (3.119)$$

$$\hat{E}_{sy,z}|^{n+1} = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} e_{sy,z}|^{n+1} - \hat{E}_{sy,z}|^{n+\frac{1}{2}} \quad (3.120)$$

$$\hat{H}_{sx,x}|^{n+1} = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} h_{sx,x}|^{n+1} - \hat{H}_{sx,x}|^{n+\frac{1}{2}} \quad (3.121)$$

$$\hat{H}_{sx,y}|^{n+1} = \frac{1}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} h_{sx,y}|^{n+1} - \hat{H}_{sx,y}|^{n+\frac{1}{2}} \quad (3.122)$$

$$\hat{H}_{sy,x}|^{n+1} = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} h_{sy,x}|^{n+1} - \hat{H}_{sy,x}|^{n+\frac{1}{2}} \quad (3.123)$$

$$\hat{H}_{sy,y}|^{n+1} = \frac{1}{\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}} h_{sy,y}|^{n+1} - \hat{H}_{sy,y}|^{n+\frac{1}{2}} \quad (3.124)$$

Output

$$E_{sx,z}|^{n+1} = \left(\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}\right) \hat{E}_{sx,z}|^{n+1}, \quad E_{sy,z}|^{n+1} = \left(\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}\right) \hat{E}_{sy,z}|^{n+1} \quad (3.125)$$

$$H_{sx,x}|^{n+1} = \left(\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}\right) \hat{H}_{sx,x}|^{n+1}, \quad H_{sx,y}|^{n+1} = \left(\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}\right) \hat{H}_{sx,y}|^{n+1} \quad (3.126)$$

$$H_{sy,x}|^{n+1} = \left(\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}\right) \hat{H}_{sy,x}|^{n+1}, \quad H_{sy,y}|^{n+1} = \left(\frac{1}{2} + \frac{\sigma_y \Delta t}{8\epsilon_0}\right) \hat{H}_{sy,y}|^{n+1}. \quad (3.127)$$

Next, we discuss the actual numerical update of $\hat{\mathbf{u}}$. For spatial discretization, we consider Yee's grid with inhomogeneous media and split-field components $\{E_{sx,z}, E_{sy,z}\}$, $\{H_{sx,x}, H_{sy,x}\}$ and $\{H_{sx,y}, H_{sy,y}\}$ located at positions (i, j) , $(i, j + \frac{1}{2})$ and $(i + \frac{1}{2}, j)$, respectively. Consider Substep 1 as an illustration. First, the update of auxiliary field vector $\mathbf{v}^{n+\frac{1}{2}}$ is performed via (3.101)-(3.106). The auxiliary field component $e_{sx,z}|_{i,j}^{n+\frac{1}{2}}$ is first updated implicitly by solving a system of linear equations of form

$$\begin{aligned} & -\beta|_{i,j} \gamma^{yy}|_{i-\frac{1}{2},j} e_{sx,z}|_{i-1,j}^{n+\frac{1}{2}} + (1 + \beta|_{i,j} \gamma^{yy}|_{i-\frac{1}{2},j} + \beta|_{i,j} \gamma^{yy}|_{i+\frac{1}{2},j}) e_{sx,z}|_{i,j}^{n+\frac{1}{2}} \\ & -\beta|_{i,j} \gamma^{yy}|_{i+\frac{1}{2},j} e_{sx,z}|_{i+1,j}^{n+\frac{1}{2}} \\ & = \hat{E}_{sx,z}|_{i,j}^n + \beta|_{i,j} \gamma^{yy}|_{i-\frac{1}{2},j} \hat{E}_{sy,z}|_{i-1,j}^n - (\beta|_{i,j} \gamma^{yy}|_{i-\frac{1}{2},j} + \beta|_{i,j} \gamma^{yy}|_{i+\frac{1}{2},j}) \hat{E}_{sy,z}|_{i,j}^n \\ & + \beta|_{i,j} \gamma^{yy}|_{i+\frac{1}{2},j} \hat{E}_{sy,z}|_{i+1,j}^n + \beta|_{i,j} (\hat{H}_{sx,y}|_{i+\frac{1}{2},j}^n + \hat{H}_{sy,y}|_{i+\frac{1}{2},j}^n - \hat{H}_{sx,y}|_{i-\frac{1}{2},j}^n - \hat{H}_{sy,y}|_{i-\frac{1}{2},j}^n), \end{aligned} \quad (3.128)$$

with tridiagonal matrix coefficient. Equation (3.128) can be attained by first substituting $e_{sy,z}|_{i,j}^{n+\frac{1}{2}} = \hat{E}_{sy,z}|_{i,j}^n$ and $h_{sy,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \hat{H}_{sy,y}|_{i+\frac{1}{2},j}^n$ into the RHSs of implicit update equations for $h_{sx,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$ and $e_{sx,z}|_{i,j}^{n+\frac{1}{2}}$, respectively. The RHS of update equation $h_{sx,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$ is then substituted into the update equation of $e_{sx,z}|_{i,j}^{n+\frac{1}{2}}$. In (3.128), $\beta|_{i,j}$ and $\gamma^{yy}|_{i+\frac{1}{2},j}$ are

$$\beta|_{i,j} = \frac{\frac{\Delta t}{4\epsilon_r|_{i,j}\epsilon_0\Delta x}}{\frac{1}{2} + \frac{\sigma_x|_{i,j}\Delta t}{8\epsilon_0}} \quad \text{and} \quad \gamma^{yy}|_{i+\frac{1}{2},j} = \frac{\frac{v_{yyr}|_{i+\frac{1}{2},j}\Delta t}{4\mu_0\Delta x}}{\frac{1}{2} + \frac{\sigma_x|_{i+\frac{1}{2},j}\Delta t}{8\epsilon_0}}.$$

The inhomogeneity in anisotropic media is effectively incorporated in the terms of $\beta|_{i,j}$ and $\gamma^{yy}|_{i+\frac{1}{2},j}$. With $e_{sx,z}|_{i,j}^{n+\frac{1}{2}}$ solved, the remaining fields can be updated explicitly using

$$h_{sx,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \hat{H}_{sx,y}|_{i+\frac{1}{2},j}^n + \gamma^{yy}|_{i+\frac{1}{2},j}(e_{sx,z}|_{i+1,j}^{n+\frac{1}{2}} - e_{sx,z}|_{i,j}^{n+\frac{1}{2}} + \hat{E}_{sy,z}|_{i+1,j}^n - \hat{E}_{sy,z}|_{i,j}^n) \quad (3.129)$$

$$h_{sx,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \hat{H}_{sx,x}|_{i,j+\frac{1}{2}}^n + \left\{ \frac{\mathbf{v}_{xyr}}{\mathbf{v}_{yyr}} (h_{sx,y}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{H}_{sx,y}|_{i,j+\frac{1}{2}}^n) \right\}_{i,j+\frac{1}{2}} \quad (3.130)$$

$$e_{sy,z}|_{i,j}^{n+\frac{1}{2}} = \hat{E}_{sy,z}|_{i,j}^n \quad (3.131)$$

$$h_{sy,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \hat{H}_{sy,x}|_{i,j+\frac{1}{2}}^n \quad (3.132)$$

$$h_{sy,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \hat{H}_{sy,y}|_{i+\frac{1}{2},j}^n. \quad (3.133)$$

Note that update (3.130) for $h_{sx,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}$ includes a non-diagonal term from the anisotropic permeability tensor. It is attained by first substituting for the term

$$\frac{\frac{\Delta t}{4\mu_0}}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} \left(\frac{\partial e_{sx,z}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}}{\partial x} + \frac{\partial e_{sy,z}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}}{\partial x} \right)$$

in (3.103) with the RHS attained from (3.104) as

$$\frac{\frac{\Delta t}{4\mu_0}}{\frac{1}{2} + \frac{\sigma_x \Delta t}{8\epsilon_0}} \left(\frac{\partial e_{sx,z}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}}{\partial x} + \frac{\partial e_{sy,z}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}}{\partial x} \right) = \frac{1}{\mathbf{v}_{yyr}} (h_{sx,y}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{H}_{sx,y}|_{i,j+\frac{1}{2}}^n).$$

and then sampling it at $(i, j + \frac{1}{2})$. A similar equation is presented for the non-PML case in (3.27). As the fields $h_{sx,y}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}$ and $\hat{H}_{sx,y}|_{i,j+\frac{1}{2}}^n$ are not available at $(i, j + \frac{1}{2})$, they have to be interpolated from neighboring points. The interpolation is performed in a similar manner as that for the non-PML case. Upon the update of auxiliary field vector $\mathbf{v}^{n+\frac{1}{2}}$, the intermediate field vector $\hat{\mathbf{u}}^{n+\frac{1}{2}}$ can be updated directly and explicitly by using (3.107)-(3.112). Note that further efficiencies can be attained by combining the auxiliary field updates (3.131)-(3.133) with the corresponding intermediate field updates in (3.108) and

(3.111)-(3.112), respectively as

$$\begin{aligned}\hat{E}_{sy,z}|_{i,j}^{n+\frac{1}{2}} &= \frac{1}{\frac{1}{2} + \frac{\sigma_y|_{i,j}\Delta t}{8\epsilon_0}} e_{sy,z}|_{i,j}^{n+\frac{1}{2}} - \hat{E}_{sy,z}|_{i,j}^n \\ &= \left(\frac{1}{\frac{1}{2} + \frac{\sigma_y|_{i,j}\Delta t}{8\epsilon_0}} - 1 \right) \hat{E}_{sy,z}|_{i,j}^n\end{aligned}\quad (3.134)$$

$$\begin{aligned}\hat{H}_{sy,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{\frac{1}{2} + \frac{\sigma_y|_{i,j+\frac{1}{2}}\Delta t}{8\epsilon_0}} h_{sy,x}|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{H}_{sy,x}|_{i,j+\frac{1}{2}}^n \\ &= \left(\frac{1}{\frac{1}{2} + \frac{\sigma_y|_{i,j+\frac{1}{2}}\Delta t}{8\epsilon_0}} - 1 \right) \hat{H}_{sy,x}|_{i,j+\frac{1}{2}}^n\end{aligned}\quad (3.135)$$

$$\begin{aligned}\hat{H}_{sy,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} &= \frac{1}{\frac{1}{2} + \frac{\sigma_y|_{i+\frac{1}{2},j}\Delta t}{8\epsilon_0}} h_{sy,y}|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - \hat{H}_{sy,y}|_{i+\frac{1}{2},j}^n \\ &= \left(\frac{1}{\frac{1}{2} + \frac{\sigma_y|_{i+\frac{1}{2},j}\Delta t}{8\epsilon_0}} - 1 \right) \hat{H}_{sy,y}|_{i+\frac{1}{2},j}^n.\end{aligned}\quad (3.136)$$

Following the above, a similar set of update procedure can be deduced for Substep 2 to complete the update of final field vector $\hat{\mathbf{u}}^{n+1}$.

3.3 Stability Analysis

In this section, we analyze the stability of the proposed split-step FDTD method for 3-D Maxwell's equations in general anisotropic media. Due to the complexity, there is not much literature for stability analysis in general anisotropic media. Hence, we resort to the Fourier method and numerically investigate the eigenvalues of the Fourier amplification matrix.

Let the 6×6 amplification matrix of each substep be denoted as $\mathbf{G}_i$, where i is the substep number ranging from 1 to 6, and the amplification matrix of the entire update from n to $n+1$ be denoted as $\mathbf{G}$. The amplification matrix $\mathbf{G}_i$ is determined from the

proposed split-step FDTD formulation in terms of $\mathbf{E}$ - $\mathbf{H}$ field components. The computation of amplification matrices $\mathbf{G}_i$ and $\mathbf{G}$ are presented in the Appendix A. Note that some elements of amplification matrix $\mathbf{G}_i$ contain certain cosine terms. These cosine terms arise upon Fourier transformation of field components as determined by the interpolation operation described earlier, cf. (3.61). The relationship between amplification matrix $\mathbf{G}$ and the field vector in Fourier domain is written as

$$\mathbf{U}^{n+1} = \mathbf{G}\mathbf{U}^n \quad (3.137)$$

where $\mathbf{G} = \mathbf{G}_6\mathbf{G}_5\mathbf{G}_4\mathbf{G}_3\mathbf{G}_2\mathbf{G}_1$ and $\mathbf{U}$ is the 6×1 field vector in Fourier domain,

$$\mathbf{U} = \begin{bmatrix} E_{xo} & E_{yo} & E_{zo} & H_{xo} & H_{yo} & H_{zo} \end{bmatrix}^T. \quad (3.138)$$

To analyze the stability of the proposed split-step FDTD method, we numerically scan the eigenvalues of the amplification matrix $\mathbf{G}$ over a range of Fourier wavenumbers. In this numerical scan, we consider three arbitrary cases of anisotropic media, namely, electric, magnetic and general (both electric and magnetic) anisotropic media and denote them as anisotropic medium 1 ($\bar{\bar{\epsilon}} = \bar{\bar{\epsilon}}_r \epsilon_0$ and $\bar{\bar{\mu}} = \mathbf{I} \mu_0$), medium 2 ($\bar{\bar{\epsilon}} = \mathbf{I} \epsilon_0$ and $\bar{\bar{\mu}} = \bar{\bar{\mu}}_r \mu_0$) and medium 3 ($\bar{\bar{\epsilon}} = \bar{\bar{\epsilon}}_r \epsilon_0$ and $\bar{\bar{\mu}} = \bar{\bar{\mu}}_r \mu_0$), respectively, with

$$\bar{\bar{\epsilon}}_r = \begin{bmatrix} 10.225 & -0.825 & -0.55\sqrt{\frac{3}{2}} \\ -0.825 & 10.225 & 0.55\sqrt{\frac{3}{2}} \\ -0.55\sqrt{\frac{3}{2}} & 0.55\sqrt{\frac{3}{2}} & 9.95 \end{bmatrix}$$

$$\bar{\bar{\mu}}_r = \begin{bmatrix} 3.75 & 0.75 & -0.5\sqrt{\frac{3}{2}} \\ 0.75 & 3.75 & -0.5\sqrt{\frac{3}{2}} \\ -0.5\sqrt{\frac{3}{2}} & -0.5\sqrt{\frac{3}{2}} & 3.5 \end{bmatrix}.$$

ϵ_0 and μ_0 are the free space permittivity and permeability, respectively. We assume uniform cell size $\Delta x = \Delta y = \Delta z = \Delta$ of 6.255mm, 1.033mm and 1.615mm for the case of medium 1, 2 and 3, respectively. We denote the Courant-limit time step as $\Delta t_{CFL} = \frac{\Delta}{c\sqrt{3}}$ where c is the speed of light in free space.

The eigenvalues of the amplification matrix $\mathbf{G}$ for medium 1, 2 and 3 are scanned over four independent parameters, namely the time step size $\Delta t = \text{CFLN} \Delta t_{CFL}$ where CFLN is the Courant number and the angles θ_x , θ_y and θ_z , which are related to the Fourier wavenumbers k_x , k_y and k_z (see Appendix A). The CFLN number is set to 1, 5, 10, 20, 60 and 100. The angles θ_x , θ_y and θ_z are each set to values across a range of 0 to 2π radians and interval of 0.15 radians. For each medium case and CFLN value, we determine amplification matrices $\mathbf{G}$ and their corresponding eigenvalues. These eigenvalues are plotted on the unit semicircle and shown in Figs. 3.1(a)-3.1(c).

From the figures, we observe that, for $\text{CFLN} \geq 1$, the eigenvalues corresponding to anisotropic medium 1, 2 and 3 still lie on the unit semicircle and have unity magnitude, thereby illustrating the stable and non-dissipative nature of the proposed split-step FDTD method for 3-D Maxwell's equation in general anisotropic media.

(a) Case of medium 1 (electric anisotropic)

(b) Case of medium 2 (magnetic anisotropic)

(c) Case of medium 3 (general anisotropic)

Figure 3.1: Eigenvalues (dots) of amplification matrix $\mathbf{G}$ around unit semicircle for various medium cases.

3.4 Numerical Results

In this section, we present numerical results from five experiments to validate the stability, accuracy and efficiency of the proposed split-step FDTD method for 3-D Maxwell's equations in general anisotropic media. For these experiments, the proposed methods are generally coded sequentially in both Matlab as well as C++ environments. To obtain central processing unit time, C++ environment is used.

3.4.1 Experiment 1: 3-D Cavity with Homogeneous Anisotropic Media

In experiment 1, we simulate a $30 \times 30 \times 30$ uniform grid rectangular cavity filled with homogeneous anisotropic medium characterized by medium 1, 2 and 3 in Section 3.3 and with perfect electric conducting (PEC) boundary conditions. We assume uniform cell size (Δ) of 0.447mm, 1.033mm and 1.615mm for anisotropic medium 1, 2 and 3, respectively. These cell sizes correspond to cell per minimum wavelength (N_λ) of 40, 38 and 23, respectively. The minimum wavelengths in the anisotropic media are approximated using the relation $\frac{\lambda_{3dB}}{\sqrt{\epsilon_{r,max}\mu_{r,max}}}$, where $\epsilon_{r,max}$ and $\mu_{r,max}$ are the maximum absolute elements from $\bar{\bar{\epsilon}}_r$ and $\bar{\bar{\mu}}_r$, respectively, and λ_{3dB} is the free space wavelength corresponding to the upper -3 dB frequency of the source function. The source function is modeled by a bandpass Gaussian function: $\sin(\omega_0(t - t_0))e^{-(\frac{t-t_0}{\tau})^2}$ where $\omega_0 = 9.4\pi \times 10^9 \text{ rad/s}$, $7.088\pi \times 10^9 \text{ rad/s}$ and $2.286\pi \times 10^9 \text{ rad/s}$, $t_0 = n_0\Delta t_{CFL}$ with $n_0 = 1500, 1000$ and 1000 and $\tau = m\Delta t_{CFL}$ with $m = 520, 225$ and 322 for case of medium 1, 2 and 3, respectively. The magnetic current source is applied to the H_z field at source point (16,25,16).

Figure 3.2: Example of H_z field update on PEC boundary $z = 0$ in Substep 1.

The experiment uses a Yee's grid, in which, the tangential electric field and normal magnetic field components lie on the PEC boundaries. Due to PEC boundary condition, the electric field components on the PEC boundaries are explicitly set to zero. The normal magnetic field components may be nonzero, for the case of medium characterized by anisotropic permeability tensor, although the normal magnetic flux components are set to zero. To update the normal magnetic field components on the PEC boundaries, we utilize image theory [98] along with the formulae in the proposed split-step FDTD method. As an illustration, consider the update of the normal magnetic field component $H_z|_{i+\frac{1}{2},j+\frac{1}{2},0}^{n,1}$ in Substep 1 on the PEC boundary $z = 0$. Using (3.28), we can compute $H_z|_{i+\frac{1}{2},j+\frac{1}{2},0}^{n,1}$ as

$$H_z|_{i+\frac{1}{2},j+\frac{1}{2},0}^{n,1} = \frac{v_{zy}}{v_{yy}}(H_y|_{i+\frac{1}{2},j+\frac{1}{2},0}^{n,1} - H_y|_{i+\frac{1}{2},j+\frac{1}{2},0}^n) + H_z|_{i+\frac{1}{2},j+\frac{1}{2},0}^n. \quad (3.139)$$

The H_y fields in (3.139) are interpolated to $H_z(i + \frac{1}{2}, j + \frac{1}{2}, 0)$ position using

$$H_y|_{i+\frac{1}{2}, j+\frac{1}{2}, 0} = \frac{1}{4}(H_y|_{i+\frac{1}{2}, j, \frac{1}{2}} + H_y|_{i+\frac{1}{2}, j+1, \frac{1}{2}} + H_y|_{i+\frac{1}{2}, j, -\frac{1}{2}} + H_y|_{i+\frac{1}{2}, j+1, -\frac{1}{2}}). \quad (3.140)$$

This is also shown in Fig. 3.2, where H_z and neighboring H_y fields are highlighted in red and blue, respectively. As shown in Fig. 3.2, two of the neighboring H_y fields, namely, $H_y|_{i+\frac{1}{2}, j, -\frac{1}{2}}$ and $H_y|_{i+\frac{1}{2}, j+1, -\frac{1}{2}}$ lie outside the cavity region. Using image theory [98], we equate them to fields inside the cavity as $H_y|_{i+\frac{1}{2}, j, -\frac{1}{2}} = H_y|_{i+\frac{1}{2}, j, \frac{1}{2}}$ and $H_y|_{i+\frac{1}{2}, j+1, -\frac{1}{2}} = H_y|_{i+\frac{1}{2}, j+1, \frac{1}{2}}$. Substituting these relations in (3.140) we can compute H_y on the $z = 0$ PEC boundary as

$$H_y|_{i+\frac{1}{2}, j+\frac{1}{2}, 0} = \frac{1}{4}(2H_y|_{i+\frac{1}{2}, j, \frac{1}{2}} + 2H_y|_{i+\frac{1}{2}, j+1, \frac{1}{2}}). \quad (3.141)$$

Once $H_y|_{i+\frac{1}{2}, j+\frac{1}{2}, 0}^{n,1}$ on the PEC boundary is known, $H_z|_{i+\frac{1}{2}, j+\frac{1}{2}, 0}^{n,1}$ can be computed using (3.139). This approach is similarly used to solve for other normal magnetic field components on the PEC boundaries. With the tangential electric field and normal magnetic field components on the PEC boundaries deduced, the remaining fields within cavity can be solved.

At observation point (16,7,7) the time domain H_z field is first recorded over 10000, 5000 and 7500 iterations for experiment with anisotropic medium 1, 2 and 3, respectively. For each medium case, the experiment is repeated using the proposed split-step FDTD method with CFLN values, ranging from 1 to 10. The experimental results are compared with the explicit FDTD method for anisotropic media [28]-[34] at CFLN=1. Plots of the normalized H_z field using the proposed split-step FDTD method at CFLN=10 and the explicit FDTD method are shown in Figs. 3.3(a)-3.3(c). The figures show stable time domain H_z fields using the proposed split-step FDTD method for

Table 3.1: Comparison of CPU time between proposed split-step FDTD and explicit FDTD for Experiment 1

Method	Δt	Time Steps	CPU Time
Explicit FDTD	3.11 ps	100000	700.56 s
Split-Step FDTD (CFLN=1)	3.11 ps	100000	2481.52 s
Split-Step FDTD (CFLN=3)	9.33 ps	33333	827.51 s
Split-Step FDTD (CFLN=4)	12.44 ps	25000	619.05 s
Split-Step FDTD (CFLN=8)	24.88 ps	12500	309.88 s
Split-Step FDTD (CFLN=10)	31.10 ps	10000	248.28 s

all media cases. Good agreement is also shown between the proposed split-step FDTD method and the explicit FDTD method.

(a) Case of medium 1 (electric anisotropic)

(b) Case of medium 2 (magnetic anisotropic)

(c) Case of medium 3 (general anisotropic)

Figure 3.3: Time-domain H_z computed using Split-Step FDTD (CFLN=10) and Explicit FDTD for various medium cases.

Figure 3.4: Resonant frequencies extracted using Split-Step FDTD and Explicit FDTD for case of medium 3 (general anisotropic). Top and bottom plots correspond to resonance at 1.257 GHz and 1.187 GHz, respectively.

The resonant frequencies are next extracted from the time domain H_z fields, recorded over longer iterations of 100000 time steps. The required central processing unit (CPU) time of the proposed split-step FDTD method at various CFLNs and the explicit FDTD method is compared in Table 3.1 for the case of medium 3. The computing platform is C++ environment with Intel Dual Core 3.00 GHz processor. From the table, we observe that the proposed split-step FDTD method achieves a lower CPU time and is computationally efficient compared to the explicit FDTD method for $\text{CFLN} \geq 4$. However, the price to pay for this efficiency is a reduction in accuracy that can be observed from the resonant frequency versus CFLN plots in Fig. 3.4. The top and bottom plots in Fig. 3.4 correspond to the resonant frequencies 1.257 GHz and 1.187 GHz, respectively. From the figures, we observe that the relative frequency error between the proposed split-step FDTD method and the explicit FDTD method increases as CFLN increases. Specifically, the relative errors at $\text{CFLN}=10$ are 0.32% and 0.28% for the resonant frequencies 1.257 GHz and 1.187 GHz, respectively. The resonant frequencies extracted using the proposed split-step FDTD method is still in good agreement with the explicit FDTD method. Similarly, good agreement is observed for cases of medium 1 and 2.

Figure 3.5: Time-domain H_z computed using Split-Step FDTD (CFLN=100) over 80000 iterations for case of medium 3 (general anisotropic).

Next, we validate the late time stability of the proposed split-step FDTD method. A point source is initialized at the H_z field at source point (16,25,16). At observation point (16,7,7) the time domain H_z field is recorded over 80000 iterations with CFLN=100 (which corresponds to 8 million time steps at CFLN=1) for case of medium 3. In Fig. 3.5, we plot the normalized H_z field using the proposed split-step FDTD method with CFLN=100. From the figure, we observe stable time domain H_z field even after large number of iterations. Late time stable results were similarly observed for smaller CFLN and for cases of medium 1 and 2.

3.4.2 Experiment 2: 3-D Cavity with Anisotropic Dielectric Resonator

In experiment 2, we simulate a $30 \times 30 \times 30$ uniform grid rectangular cavity with a centered $24 \times 24 \times 22$ anisotropic dielectric resonator surrounded by air and with PEC boundary condition, as illustrated in Fig. 3.6 inset (xz plane view). Anisotropic dielectric resonator in cavities have previously been investigated in [99] using the finite

Table 3.2: Comparison of CPU time between proposed split-step FDTD and explicit FDTD for Experiment 2

Method	Δt	Time Steps	CPU Time
Explicit FDTD	12.04 ps	8000	46.093 s
Split-Step FDTD (CFLN=1)	12.04 ps	8000	159.746 s
Split-Step FDTD (CFLN=3)	36.14 ps	2667	53.545 s
Split-Step FDTD (CFLN=4)	48.18 ps	2000	40.014 s
Split-Step FDTD (CFLN=8)	96.36 ps	1000	20.140 s
Split-Step FDTD (CFLN=10)	120.45 ps	800	16.093 s

element method to extract resonant modes. Here, we investigate the resonant modes extracted using the proposed split-step FDTD method. The anisotropic dielectric resonator is characterized by medium 1 of Section 3.3. We assume uniform cell size of 6.255mm that corresponds to $N_\lambda = 21$. The source function is modeled by a bandpass Gaussian function: $\sin(\omega_0(t - t_0))e^{-(\frac{t-t_0}{\tau})^2}$ with $\omega_0 = 1.0844\pi \times 10^9 \text{ rad/s}$, $t_0 = 800\Delta t_{CFL}$ and $\tau = 83\Delta t_{CFL}$. The current source is applied to the E_z field at source point (10,10,15).

At observation point (22,22,22), the time domain E_z field is recorded over 8000 iterations using the explicit FDTD method and the proposed split-step FDTD method with CFLN values ranging from 1 to 10. The required CPU time of the proposed split-step FDTD method at various CFLNs and the explicit FDTD method is compared in Table 3.2. From the table, we observe that the proposed split-step FDTD method achieves a lower CPU time and is computationally efficient compared to the explicit FDTD method for $\text{CFLN} \geq 4$.

The accuracy of the proposed split-step FDTD method is next analyzed. We first compare the magnitude of the E_z field in frequency domain using the proposed split-step FDTD method at CFLN=5 and the explicit FDTD method. This comparison is shown in Fig. 3.6. From the figure, we observe reasonably good agreement between

Figure 3.6: Magnitude of $E_z(\omega)$ versus frequency computed using Split-Step FDTD (CFLN=5) and Explicit FDTD for case of medium 1 (electric anisotropic) dielectric resonator.

Figure 3.7: Resonant frequencies extracted using Split-Step FDTD and Explicit FDTD for case of anisotropic dielectric resonator. Top and bottom plots correspond to resonance at 6.48×10^8 Hz and 7.78×10^8 Hz, respectively.

both methods. Next, we compare the resonant frequencies extracted using the explicit FDTD method and the proposed split-step FDTD method with CFLN ranging from 1 to 10. This comparison is highlighted in Fig. 3.7, where the top and bottom plots correspond to the resonance at 6.48×10^8 Hz and 7.78×10^8 Hz, respectively. From the

Figure 3.8: Time-domain scattered E_y computed using Split-Step FDTD (CFLN=1, 5 and 10) and Explicit FDTD.

figure, we observe that the relative errors at CFLN=10 are 1.63% and 2.56% for the resonant frequencies 6.48×10^8 Hz and 7.78×10^8 Hz, respectively. The resonant frequencies extracted by both methods are still in good agreement. Fig. 3.7 also illustrates that the maximum tolerable error levels of 1%, 2% and 3% can be met by operating the proposed split-step FDTD method with CFLN of 5, 8 and 10, respectively.

3.4.3 Experiment 3: 3-D Scattering from Anisotropic Dielectric Cube

In experiment 3, we simulate 3-D scattering from a $40 \times 40 \times 40$ uniform grid anisotropic dielectric cube centered in a $100 \times 100 \times 100$ computational domain. The anisotropic dielectric cube and background media are characterized by medium 1 of Section 3.3 and free space, respectively. We assume uniform cell size of 2mm that corresponds to $N_\lambda = 40$. The total-field/scattered-field (TF/SF) formulation is used to introduce into the total-field region a y -polarized incident plane wave, propagating towards the positive x

direction [97]. The incident plane wave is modeled using a bandpass Gaussian pulse: $\sin(\omega_0(t - t_0))e^{-(\frac{t-t_0}{\tau})^2}$ with $\omega_0 = 2\pi \times 10^9 \text{ rad/s}$, $t_0 = 750\Delta t_{CFL}$ and $\tau = 308\Delta t_{CFL}$. The Mur absorbing boundary condition (ABC) [73], [100] is used to terminate the boundaries of the computational domain. The cross sectional view of the computational domain is shown in Fig. 3.8 inset.

At the observation point (90,90,51), in the scattered-field region, the scattered E_y field is recorded over 5000 iterations using the explicit FDTD method and proposed split-step FDTD method with CFLN of 1, 5 and 10. The normalized scattered E_y field extracted by both methods are plotted and compared in Fig. 3.8. From the figure, we observe that as the CFLN increases from 1 to 10 (time step size increases from Δt_{CFL} to $10\Delta t_{CFL}$ and number of iterations reduces from 5000 to 500), the matching of time-domain field plots with the explicit FDTD method slightly degrades but is still acceptable. This signifies the trade-off between efficiency and accuracy of the split-step FDTD method.

3.4.4 Experiment 4: 2-D Scattering from Anisotropic Dielectric Cylinder

In experiment 4, we verify 2-D simulation with TE_z (E_x , E_y and H_z) scattering from an infinitely long anisotropic dielectric cylinder of radius 40 grids, centered in a 200×200 uniform computational domain. Fig. 3.9 illustrates the fine-grid staircase modeling of the dielectric cylinder. The anisotropic dielectric cylinder is characterized by a relative permittivity tensor

$$\bar{\epsilon}_r = \begin{bmatrix} 6.5 & 2.1 \\ 2.1 & 6.5 \end{bmatrix}$$

Figure 3.9: Fine-grid staircase mesh of dielectric cylinder.

and free space permeability. The background media is free space. We assume uniform cell size of 2.5mm that corresponds to $N_\lambda = 41$. The TF/SF formulation is used to introduce into the total-field region a y -polarized incident plane wave, propagating towards the positive x direction. The incident plane wave is modeled using a bandpass Gaussian pulse: $\sin(\omega_0(t - t_0))e^{-\left(\frac{t-t_0}{\tau}\right)^2}$ with $\omega_0 = 2\pi \times 10^9 \text{ rad/s}$, $t_0 = 750\Delta t_{CFL,2D}$ and $\tau = 201\Delta t_{CFL,2D}$. $\Delta t_{CFL,2D}$ is the Courant-limit time step size in a 2-D free space grid. The Mur ABC is used to terminate the boundaries of the computational domain. After 10000 iterations, the bistatic radar cross section (RCS) is determined from the scattered-fields in the scattered-field region. Fig. 3.10 compares the RCS extracted using the proposed split-step FDTD method with CFLN of 1 and 5 and the explicit FDTD method. From the figure, we observe good agreement between both methods.

Figure 3.10: Radar cross section (dB) computed using Split-Step FDTD (CFLN=1 and 5) and Explicit FDTD.

3.4.5 Experiment 5: 2-D Tunable Anisotropic Photonic Crystal Cavity

In experiment 5, we validate the split-step FDTD method with PML boundary conditions, as proposed in Section 3.2.3. We consider an example of a 2-D tunable photonic crystal (PhC) cavity with anisotropic media. Anisotropic media can be used in the form of localized defects to tune frequency of defect modes in PhC devices such as cavities and filters [101]-[103]. Such anisotropic media include liquid crystals [101] and ferrites [102] that have permittivity and permeability tensors tunable by external electric and magnetic fields, respectively.

Consider a 5×5 square PhC cavity consisting of dielectric rods with scalar permittivity $\epsilon = 11.56$ in air, as shown in inset of Fig. 3.11. Fig. 3.12 illustrates the fine-grid staircase modeling of each dielectric rod. The grey-shaded rods have free space permeability whereas the black-shaded rods have anisotropic permeability with tensor elements $\mu_{xx} = 1.3 \cos^2 \phi + 1.1 \sin^2 \phi$, $\mu_{yy} = 1.3 \sin^2 \phi + 1.1 \cos^2 \phi$, $\mu_{xy} = \mu_{yx} = 0.2 \sin \phi \cos \phi$. The rods have radius $r = 0.2a$ with lattice constant $a = 1.55 \mu\text{m}$. The cavity centre is

Figure 3.11: Normalized resonant frequency versus anisotropy tuning angle ϕ using explicit and split-step (denoted as SS) FDTD methods.

excited by a modulated Gaussian pulse: $\cos(\omega_c t) e^{-\left(\frac{t-t_0}{\tau}\right)^2}$ with $\omega_c = 0.3762 \frac{2\pi c_0}{a}$ (c_0 is the speed of wave in free space), $t_0 = 300\text{fs}$ and $\tau = 90\text{fs}$. The simulation runs for $\frac{300000}{\text{CFLN}}$ time steps of size $\Delta t = \text{CFLN} \frac{\Delta}{c_0 \sqrt{2}}$. A uniform cell size of $\Delta = 19.38\text{nm}$ is used, which corresponds to $N_\lambda = 44$. The simulation is terminated with 20 PML layers.

Fig. 3.11 plots the normalized resonant frequency of the PhC cavity over various tuning angles ϕ , using the explicit [56] and proposed split-step FDTD methods. From the figure, we first observe that the PhC cavity has a tunable frequency range of 0.503 THz over $\phi = 0^\circ$ to 90° with maximum tunability within $\phi = 20^\circ$ and 70° . Second, the proposed split-step FDTD methods require lower computational times compared to the explicit FDTD method, while maintaining good agreement. Specifically, at CFLN=6, the split-step FDTD method requires about 44% of the CPU time while maintaining a low maximum frequency error of 0.17% with respect to the explicit FDTD method. Fig. 3.13 further plots the E_z field in the xy plane using the proposed split-step FDTD method at CFLN=5 and $\phi = 30^\circ$. From the figure, we observe that the field is well-localized within the defect (cavity) region of the PhC.

Figure 3.12: Fine-grid staircase mesh of each cylindrical dielectric rod in PhC cavity (example shown for 1st rod from top-left).

Figure 3.13: E_z field over PhC for $\phi = 30^\circ$ using split-step FDTD method at CFLN=5. i and j coordinates are in terms of indices while unit of E_z is V/m.

3.5 Concluding Remarks

This chapter has presented a split-step FDTD method for 3-D Maxwell's equations in general anisotropic media. The general anisotropic media can be characterized by full permittivity and permeability tensors. The proposed split-step FDTD method splits the field update from n to $n + 1$ into 6 substeps. In each substep, two field components are first solved from a system of linear equations with tridiagonal coefficient matrix. These

two field components are then used in explicit update equations to determine the remaining four field components. An extension of the proposed split-step FDTD method with PML boundary conditions was further exemplified. Stability analysis of the proposed split-step FDTD method using the Fourier method was presented. The eigenvalues of the Fourier amplification matrix were numerically shown to have unity magnitude even for time steps greater than the Courant-limit time step, thereby illustrating the stable and non-dissipative nature of the proposed split-step FDTD method in general anisotropic media.

Five numerical experiments have been presented to further validate the stability and accuracy of the proposed split-step FDTD method in general anisotropic media. Closed region problems involving PEC rectangular cavities filled with homogeneous and inhomogeneous anisotropic media have been considered in experiments 1 and 2, respectively. Open region problems involving scattering off anisotropic cube and infinite cylinder have been considered in experiments 3 and 4, respectively. In experiments 2, 4 and 5, inhomogeneous problems have been considered where the inhomogeneity is separated by both straight and curved interfaces. A 2-D anisotropic photonic crystal cavity with tunable resonant frequency was considered in experiment 5. Numerical results using the proposed split-step FDTD method have shown stable fields until late time even for time steps greater than the Courant-limit time step. Furthermore, it has been shown that the proposed split-step FDTD method is generally more efficient compared to the explicit FDTD method when $CFLN \geq 4$. The proposed split-step FDTD method has also been shown to attain results that are in good agreement with the explicit FDTD method.

Chapter 4

Efficient Complex Envelope

ADI-FDTD Method for Anisotropic Periodic Media

4.1 Introduction

Periodic structures involving anisotropic media have attracted considerable interest over recent years [104]-[119]. Such structures can exhibit dispersion relations that support interesting and unique effects in electromagnetic wave propagation. For example, a magnetic photonic crystal (PhC) with unit cells composed of a ferrite layer and two misaligned anisotropic dielectric layers can display an asymmetric dispersion relation with a stationary inflection point (SIP) [104]. At the SIP frequency, electromagnetic wave propagates as a slow-wave with vanishing group velocity and amplitude growth in a particular direction and as a normal wave in the opposite direction. Some practical applications of such magnetic PhCs include parallel-plate waveguides with unidirectional

wave guiding [105] and antennas with opposite directivity patterns in the receive and transmit direction [106]. Nonmagnetic PhCs with unit cells composed of an isotropic layer and two misaligned anisotropic dielectric layers can display symmetric dispersion relations such as degenerate (DBE) and split (SBE) band edges [107]. For both these dispersion relations, electromagnetic wave can propagate with vanishing group velocity and amplitude growth at frequencies near the band edge. In addition, for the SBE PhC, good transmittance can be achieved regardless of incident wave polarization. Some practical use of nonmagnetic DBE PhCs have been explored in the form of smaller directive resonator antennas [108]. Certain bulk materials such as cholesteric liquid crystals (CLC) can exhibit dielectric anisotropy that is periodic [120]-[121], thus, acting as 1-D anisotropic periodic structures. When doped with laser dye, circularly polarized lasing near the stop band edge (where there is a high density of states) can be observed.

Recently, the complex-envelope (CE) alternating direction implicit finite-difference time-domain (ADI-FDTD) method [64] was proposed for transient analysis of nonmagnetic DBE and SBE PhCs composed of materials characterized by anisotropic dielectric permittivity tensors, without gain or dispersion. The CE-ADI-FDTD method is a suitable numerical method as it adopts the ADI algorithm [26] to remove the Courant-limit time step bound, that can be computational demanding especially when highly refined grids are used for modeling sharp field variations in periodic structures or when very long simulation times are required to evolve the system to steady-state. The CE-ADI-FDTD method further adopts a CE [67] formulation that has low numerical dispersion error near the carrier frequency even for large Courant numbers. Therefore, the presence of very narrow bandwidth resonances in periodic structures can allow the CE-ADI-FDTD method to operate at large Courant numbers with reasonable accuracy.

In this chapter, we extend on the CE-ADI-FDTD method for modeling anisotropic periodic structures, namely, in four ways. First, we generally formulate the CE-ADI-FDTD method for inhomogeneous saturated ferrite media with anisotropic permittivity tensor and ferrite loss. This general formulation can be used to analyze magnetic PhCs (in addition to nonmagnetic PhCs) with unit cells composed of layers characterized by anisotropic dielectric and ferrite materials. Second, we formulate a CE-ADI-FDTD method for the modeling of nonmagnetic PhCs with gain. This gain formulated CE-ADI-FDTD method can be especially useful for efficiently analyzing lasing properties of periodic structures such as cholesteric liquid crystals doped with laser dye. Third, we present a more efficient formulation of the conventional CE-ADI-FDTD method [64] for nonmagnetic PhCs without gain. Last, we present a 2-D extension of the CE-ADI-FDTD method for inhomogeneous media composed of saturated ferrite. The four contributions presented are generally formulated based on the efficient ADI splitting formulae [26] that generates update equations with fewer and simpler right-hand side (RHS) terms, making it easy and efficient to implement the CE-ADI-FDTD method.

In Section 4.2.1 we first present the formulation of the proposed CE-ADI-FDTD method for inhomogeneous saturated ferrite media with anisotropic permittivity tensor and ferrite loss. For the case of nonmagnetic media (without ferrite), proposed CE-ADI-FDTD methods are presented in Sections 4.2.2 (a) and (b) for the cases of with and without gain, respectively. For the case of nonmagnetic media without gain, an efficiency comparison is made with the conventional CE-ADI-FDTD method [64]. A 2-D extension of the CE-ADI-FDTD method is next presented in Section 4.2.3. Numerical validation is then performed in Section 4.3 for the cases of 1-D and 2-D PhC structures. Section 4.4 finally provides the conclusion.

4.2 Formulation

4.2.1 With Magnetic Media

In this section, we present the CE-ADI-FDTD formulation for inhomogeneous saturated ferrite media with anisotropic permittivity tensor and ferrite loss. Auxiliary differential equation is used to model the saturated ferrite. Consider the following set of equations that describe wave propagation in a saturated ferrite, under small signal condition and z directed dc bias magnetic field [109]:

$$\frac{\partial \mathbf{E}}{\partial t} = \bar{\bar{\kappa}} \nabla \times \mathbf{H} \quad (4.1)$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E} - \frac{\partial \mathbf{M}}{\partial t} \quad (4.2)$$

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \mu_0 (M_s \hat{\mathbf{z}} \times \mathbf{H} + \mathbf{M} \times H_0 \hat{\mathbf{z}}) + \frac{\alpha}{M_s} (M_s \hat{\mathbf{z}} \times \frac{\partial \mathbf{M}}{\partial t}), \quad (4.3)$$

where $\mathbf{E}$, $\mathbf{H}$ and $\mathbf{M}$ are the time-varying electric field, magnetic field and magnetization vectors, respectively. M_s and H_0 denote the magnitudes of saturation magnetization and dc biasing magnetic field, respectively. γ is the gyromagnetic ratio and α is the loss constant. $\bar{\bar{\kappa}}$ represents the inverse permittivity tensor ($\bar{\bar{\kappa}} = \bar{\bar{\epsilon}}^{-1}$) with elements κ_{xz} , κ_{zx} , κ_{yz} and κ_{zy} equal to zero. Assuming plane wave propagation along the z direction, (4.1)-(4.3) reduce to six equations that can be expressed as a first-order differential system in the CE form

$$\frac{\partial \tilde{\mathbf{u}}}{\partial t} = (-j\omega_c \mathbf{I} + \mathbf{M}) \tilde{\mathbf{u}}, \quad (4.4)$$

in which field envelope vector $\tilde{\mathbf{u}}$ is

$$\tilde{\mathbf{u}} = \begin{bmatrix} \tilde{E}_x & \tilde{E}_y & \tilde{H}_x & \tilde{H}_y & \tilde{M}_x & \tilde{M}_y \end{bmatrix}^T, \quad (4.5)$$

ω_c is the carrier angular-frequency, $\mathbf{I}$ is the identity matrix and matrix $\mathbf{M}$ is

$$\mathbf{M} = \begin{bmatrix} 0 & 0 & \kappa_{xy} \frac{\partial}{\partial z} & -\kappa_{xx} \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & \kappa_{yy} \frac{\partial}{\partial z} & -\kappa_{yx} \frac{\partial}{\partial z} & 0 & 0 \\ 0 & \frac{1}{\mu_0} \frac{\partial}{\partial z} & -\frac{\omega_m \alpha}{\alpha^2 + 1} & -\frac{\omega_m}{\alpha^2 + 1} & \frac{\omega_0 \alpha}{\alpha^2 + 1} & \frac{\omega_0}{\alpha^2 + 1} \\ -\frac{1}{\mu_0} \frac{\partial}{\partial z} & 0 & \frac{\omega_m}{\alpha^2 + 1} & -\frac{\omega_m \alpha}{\alpha^2 + 1} & -\frac{\omega_0}{\alpha^2 + 1} & \frac{\omega_0 \alpha}{\alpha^2 + 1} \\ 0 & 0 & \frac{\omega_m \alpha}{\alpha^2 + 1} & \frac{\omega_m}{\alpha^2 + 1} & -\frac{\omega_0 \alpha}{\alpha^2 + 1} & -\frac{\omega_0}{\alpha^2 + 1} \\ 0 & 0 & -\frac{\omega_m}{\alpha^2 + 1} & \frac{\omega_m \alpha}{\alpha^2 + 1} & \frac{\omega_0}{\alpha^2 + 1} & -\frac{\omega_0 \alpha}{\alpha^2 + 1} \end{bmatrix}, \quad (4.6)$$

which comprises differential operators $+\frac{\partial}{\partial z}$ and $-\frac{\partial}{\partial z}$ as well as terms related to ferrite media $\omega_m = \gamma \mu_0 M_s$ and $\omega_0 = \gamma \mu_0 H_0$. The field components can be obtained from their corresponding envelopes using the relation $\mathbf{u} = \Re \{ \tilde{\mathbf{u}} e^{j\omega_c t} \}$.

By splitting the matrix $(-j\omega_c \mathbf{I} + \mathbf{M})$ into two matrices $((-j\omega_c \mathbf{I} + \mathbf{M}) = \mathbf{A} + \mathbf{B})$ and using them in the fundamental ADI splitting formulae [26], a CE-ADI formulation that updates $\tilde{\mathbf{u}}$ can be attained in compact form as

$$\text{Substep 1 : } \tilde{\mathbf{v}}^n = \tilde{\mathbf{u}}^n - \tilde{\mathbf{v}}^{n-\frac{1}{2}} \quad (4.7)$$

$$\left(\frac{1}{2} \mathbf{I} - \frac{\Delta t}{4} \mathbf{A} \right) \tilde{\mathbf{u}}^{n+\frac{1}{2}} = \tilde{\mathbf{v}}^n \quad (4.8)$$

$$\text{Substep 2 : } \tilde{\mathbf{v}}^{n+\frac{1}{2}} = \tilde{\mathbf{u}}^{n+\frac{1}{2}} - \tilde{\mathbf{v}}^n \quad (4.9)$$

$$\left(\frac{1}{2} \mathbf{I} - \frac{\Delta t}{4} \mathbf{B} \right) \tilde{\mathbf{u}}^{n+1} = \tilde{\mathbf{v}}^{n+\frac{1}{2}} \quad (4.10)$$

where $\tilde{\mathbf{v}}$ is an auxiliary vector denoted as

$$\tilde{\mathbf{v}} = \begin{bmatrix} \tilde{e}_x & \tilde{e}_y & \tilde{h}_x & \tilde{h}_y & \tilde{m}_x & \tilde{m}_y \end{bmatrix}^T \quad (4.11)$$

and $\mathbf{A}$ and $\mathbf{B}$ are 6×6 matrices selected as

$$\mathbf{A} = \begin{bmatrix} -\frac{j\omega_c}{2} & 0 & \kappa_{xy} \frac{\partial}{\partial z} & 0 & 0 & 0 \\ 0 & -\frac{j\omega_c}{2} & \kappa_{yy} \frac{\partial}{\partial z} & 0 & 0 & 0 \\ 0 & \frac{1}{\mu_0} \frac{\partial}{\partial z} & -\xi_1 & -\xi_2 & \xi_3 & \xi_4 \\ 0 & 0 & \xi_2 & -\xi_1 & -\xi_4 & \xi_3 \\ 0 & 0 & \xi_5 & \xi_2 & -\xi_6 & -\xi_4 \\ 0 & 0 & -\xi_2 & \xi_5 & \xi_4 & -\xi_6 \end{bmatrix} \quad (4.12)$$

$$\mathbf{B} = \begin{bmatrix} -\frac{j\omega_c}{2} & 0 & 0 & -\kappa_{xx} \frac{\partial}{\partial z} & 0 & 0 \\ 0 & -\frac{j\omega_c}{2} & 0 & -\kappa_{yx} \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & -\xi_1 & -\xi_2 & \xi_3 & \xi_4 \\ -\frac{1}{\mu_0} \frac{\partial}{\partial z} & 0 & \xi_2 & -\xi_1 & -\xi_4 & \xi_3 \\ 0 & 0 & \xi_5 & \xi_2 & -\xi_6 & -\xi_4 \\ 0 & 0 & -\xi_2 & \xi_5 & \xi_4 & -\xi_6 \end{bmatrix} \quad (4.13)$$

The elements ξ in matrices $\mathbf{A}$ and $\mathbf{B}$ are

$$\begin{aligned} \xi_1 &= \frac{j\omega_c}{2} + \frac{\omega_m \alpha}{2(\alpha^2 + 1)} & \xi_2 &= \frac{\omega_m}{2(\alpha^2 + 1)} & \xi_3 &= \frac{\omega_0 \alpha}{2(\alpha^2 + 1)} \\ \xi_6 &= \frac{j\omega_c}{2} + \frac{\omega_0 \alpha}{2(\alpha^2 + 1)} & \xi_4 &= \frac{\omega_0}{2(\alpha^2 + 1)} & \xi_5 &= \frac{\omega_m \alpha}{2(\alpha^2 + 1)}. \end{aligned}$$

In the CE-ADI formulation (4.7)-(4.10), the entire update from n to $n+1$ is split into two substeps, n to $n + \frac{1}{2}$ and $n + \frac{1}{2}$ to $n+1$. In each substep, the auxiliary fields are first updated using explicit update equations only. The intermediate/final fields are subsequently updated using implicit/explicit update equations.

A more efficient form of (4.7)-(4.10) with simpler $\mathbf{A}$ and $\mathbf{B}$ matrices can be attained by first noting that the left-hand side matrix operators in (4.8) and (4.10) can be expressed

in a form

$$\left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{A}\right) = \begin{bmatrix} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8}\right)\mathbf{I}_{(2 \times 2)} & -\frac{\Delta t}{4}\mathbf{A}_{1,(2 \times 4)} \\ -\frac{\Delta t}{4}\mathbf{A}_{2,(4 \times 2)} & \left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{R}\right)_{(4 \times 4)} \end{bmatrix} \quad (4.14)$$

$$\left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{B}\right) = \begin{bmatrix} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8}\right)\mathbf{I}_{(2 \times 2)} & -\frac{\Delta t}{4}\mathbf{B}_{1,(2 \times 4)} \\ -\frac{\Delta t}{4}\mathbf{B}_{2,(4 \times 2)} & \left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{R}\right)_{(4 \times 4)} \end{bmatrix}, \quad (4.15)$$

in which the bracketed subscript terms denote the size of the matrices. Next, the following normalization matrix $\mathbf{G}$ is introduced as the inverse of the diagonal block matrices of (4.14)-(4.15):

$$\mathbf{G} = \begin{bmatrix} \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}\right)\mathbf{I}_{(2 \times 2)} & \mathbf{0}_{(2 \times 4)} \\ \mathbf{0}_{(4 \times 2)} & \mathbf{P}_{(4 \times 4)} \end{bmatrix} \quad (4.16)$$

in which

$$\begin{aligned} \mathbf{P}_{(4 \times 4)} &= \left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{R}\right)_{(4 \times 4)}^{-1} \\ &= \begin{bmatrix} \frac{1}{2} + \frac{\Delta t \xi_1}{4} & \frac{\Delta t \xi_2}{4} & -\frac{\Delta t \xi_3}{4} & -\frac{\Delta t \xi_4}{4} \\ -\frac{\Delta t \xi_2}{4} & \frac{1}{2} + \frac{\Delta t \xi_1}{4} & \frac{\Delta t \xi_4}{4} & -\frac{\Delta t \xi_3}{4} \\ -\frac{\Delta t \xi_5}{4} & -\frac{\Delta t \xi_2}{4} & \frac{1}{2} + \frac{\Delta t \xi_6}{4} & \frac{\Delta t \xi_4}{4} \\ \frac{\Delta t \xi_2}{4} & -\frac{\Delta t \xi_5}{4} & -\frac{\Delta t \xi_4}{4} & \frac{1}{2} + \frac{\Delta t \xi_6}{4} \end{bmatrix}^{-1} \end{aligned} \quad (4.17)$$

and $\mathbf{0}$ is the null matrix.

Matrix $\mathbf{G}$ is next left-hand multiplied throughout (4.7)-(4.10) and after some manipulations, a more efficient form of (4.7)-(4.10) can be attained as

$$\text{Substep 1 : } \hat{\mathbf{v}}^n = \mathbf{G}\tilde{\mathbf{u}}^n - \hat{\mathbf{v}}^{n-\frac{1}{2}} \quad (4.18)$$

$$\left(\mathbf{I} - \frac{\Delta t}{4}\hat{\mathbf{A}}\right)\tilde{\mathbf{u}}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^n \quad (4.19)$$

$$\text{Substep 2 : } \hat{\mathbf{v}}^{n+\frac{1}{2}} = \mathbf{G}\tilde{\mathbf{u}}^{n+\frac{1}{2}} - \hat{\mathbf{v}}^n \quad (4.20)$$

$$\left(\mathbf{I} - \frac{\Delta t}{4}\hat{\mathbf{B}}\right)\tilde{\mathbf{u}}^{n+1} = \hat{\mathbf{v}}^{n+\frac{1}{2}} \quad (4.21)$$

where the vectors $\mathbf{G}\tilde{\mathbf{v}}$ have been grouped by an auxiliary vector $\hat{\mathbf{v}} = \mathbf{G}\tilde{\mathbf{v}}$ that is denoted as

$$\hat{\mathbf{v}} = \begin{bmatrix} \hat{e}_x & \hat{e}_y & \hat{h}_x & \hat{h}_y & \hat{m}_x & \hat{m}_y \end{bmatrix}^T \quad (4.22)$$

with input initialization $\hat{\mathbf{v}}^{-\frac{1}{2}} = \mathbf{G}\tilde{\mathbf{v}}^{-\frac{1}{2}} = \mathbf{G}(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{B})\tilde{\mathbf{u}}^0$. In most cases, for zero initial fields, the input initialization need not be performed. The $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ matrices in (4.19) and (4.21), respectively, are

$$\hat{\mathbf{A}} = \begin{bmatrix} 0 & 0 & \frac{\kappa_{xy} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 \\ 0 & 0 & \frac{\kappa_{yy} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 \\ 0 & \frac{p_{11}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \\ 0 & \frac{p_{21}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \\ 0 & \frac{p_{31}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \\ 0 & \frac{p_{41}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.23)$$

$$\hat{\mathbf{B}} = \begin{bmatrix} 0 & 0 & 0 & -\frac{\kappa_{xy} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\kappa_{yx} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 \\ -\frac{p_{12}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \\ -\frac{p_{22}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \\ -\frac{p_{32}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \\ -\frac{p_{42}}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.24)$$

in which p_{lm} denote the elements of matrix $\mathbf{P}$. Note that these matrices are much simpler compared to the $\mathbf{A}$ and $\mathbf{B}$ matrices in (4.12) and (4.13). This leads to much simpler RHS terms in the update equations of (4.19) and (4.21).

Upon expansion of (4.18)-(4.21), the following set of update equations can be attained:

Substep 1

Auxiliary updating of $\hat{\mathbf{v}}^n$ in (4.18):

$$\hat{e}_x|^n = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{E}_x|^n - \hat{e}_x|^{n-\frac{1}{2}} \quad (4.25)$$

$$\hat{e}_y|^n = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{E}_y|^n - \hat{e}_y|^{n-\frac{1}{2}} \quad (4.26)$$

$$\begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^n = \mathbf{P} \begin{bmatrix} \tilde{H}_x \\ \tilde{H}_y \\ \tilde{M}_x \\ \tilde{M}_y \end{bmatrix}^n - \begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^{n-\frac{1}{2}} \quad (4.27)$$

Intermediate updating of $\tilde{\mathbf{u}}^{n+\frac{1}{2}}$ in (4.19):

$$\tilde{E}_x|^{n+\frac{1}{2}} = \hat{e}_x|^n + \left(\frac{\frac{\kappa_{xy}\Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \frac{\partial \tilde{H}_x|^{n+\frac{1}{2}}}{\partial z} \quad (4.28)$$

$$\tilde{E}_y|^{n+\frac{1}{2}} = \hat{e}_y|^n + \left(\frac{\frac{\kappa_{yy}\Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \frac{\partial \tilde{H}_x|^{n+\frac{1}{2}}}{\partial z} \quad (4.29)$$

$$\tilde{H}_x|^{n+\frac{1}{2}} = \hat{h}_x|^n + \left(\frac{p_{11}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_y|^{n+\frac{1}{2}}}{\partial z} \quad (4.30)$$

$$\tilde{H}_y|^{n+\frac{1}{2}} = \hat{h}_y|^n + \left(\frac{p_{21}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_y|^{n+\frac{1}{2}}}{\partial z} \quad (4.31)$$

$$\tilde{M}_x|^{n+\frac{1}{2}} = \hat{m}_x|^n + \left(\frac{p_{31}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_y|^{n+\frac{1}{2}}}{\partial z} \quad (4.32)$$

$$\tilde{M}_y|^{n+\frac{1}{2}} = \hat{m}_y|^n + \left(\frac{p_{41}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_y|^{n+\frac{1}{2}}}{\partial z} \quad (4.33)$$

Substep 2

Auxiliary updating of $\hat{\mathbf{v}}^{n+\frac{1}{2}}$ in (4.20):

$$\hat{e}_x|^{n+\frac{1}{2}} = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right)\tilde{E}_x|^{n+\frac{1}{2}} - \hat{e}_x|^n \quad (4.34)$$

$$\hat{e}_y|^{n+\frac{1}{2}} = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right)\tilde{E}_y|^{n+\frac{1}{2}} - \hat{e}_y|^n \quad (4.35)$$

$$\begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^{n+\frac{1}{2}} = \mathbf{P} \begin{bmatrix} \tilde{H}_x \\ \tilde{H}_y \\ \tilde{M}_x \\ \tilde{M}_y \end{bmatrix}^{n+\frac{1}{2}} - \begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^n \quad (4.36)$$

Final updating of $\tilde{\mathbf{u}}^{n+1}$ in (4.21):

$$\tilde{E}_x|^{n+1} = \hat{e}_x|^{n+\frac{1}{2}} - \left(\frac{\kappa_{xx}\Delta t}{4}\right)\frac{\partial\tilde{H}_y|^{n+1}}{\partial z} \quad (4.37)$$

$$\tilde{E}_y|^{n+1} = \hat{e}_y|^{n+\frac{1}{2}} - \left(\frac{\kappa_{yx}\Delta t}{4}\right)\frac{\partial\tilde{H}_y|^{n+1}}{\partial z} \quad (4.38)$$

$$\tilde{H}_x|^{n+1} = \hat{h}_x|^{n+\frac{1}{2}} - \left(\frac{p_{12}\Delta t}{4\mu_0}\right)\frac{\partial\tilde{E}_x|^{n+1}}{\partial z} \quad (4.39)$$

$$\tilde{H}_y|^{n+1} = \hat{h}_y|^{n+\frac{1}{2}} - \left(\frac{p_{22}\Delta t}{4\mu_0}\right)\frac{\partial\tilde{E}_x|^{n+1}}{\partial z} \quad (4.40)$$

$$\tilde{M}_x|^{n+1} = \hat{m}_x|^{n+\frac{1}{2}} - \left(\frac{p_{32}\Delta t}{4\mu_0}\right)\frac{\partial\tilde{E}_x|^{n+1}}{\partial z} \quad (4.41)$$

$$\tilde{M}_y|^{n+1} = \hat{m}_y|^{n+\frac{1}{2}} - \left(\frac{p_{42}\Delta t}{4\mu_0}\right)\frac{\partial\tilde{E}_x|^{n+1}}{\partial z} \quad (4.42)$$

The actual numerical update of components of $\tilde{\mathbf{u}}$ is next discussed. For spatial discretization, we assume grid cells of size Δz with staggered $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{H}}$ and collocated $\tilde{\mathbf{H}}$ and $\tilde{\mathbf{M}}$ field positions. To cater for inhomogeneity in media, update coefficients are explicitly sampled at either k or $k + \frac{1}{2}$ positions (denoted as subscripts), which correspond to $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{H}}$ field positions, respectively. Consider the Substep 1 as an illustration. First, the update of auxiliary fields $\hat{\mathbf{v}}^n$ is directly determined using explicit update equations

(4.25)-(4.27). Next, the update of intermediate fields $\tilde{\mathbf{u}}^{n+\frac{1}{2}}$ is performed using (4.28)-(4.33). In this part, the implicit update of $\tilde{E}_y|_k^{n+\frac{1}{2}}$ is first attained from a system of linear equations in the form

$$\begin{aligned}
& -\left(\frac{p_{11}\Delta t}{4\mu_0\Delta z}\right)|_{k-\frac{1}{2}}\left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2}+\frac{j\omega_c\Delta t}{8}}\right)|_k\tilde{E}_y|_{k-\frac{1}{2}}^{n+\frac{1}{2}}-\left(\frac{p_{11}\Delta t}{4\mu_0\Delta z}\right)|_{k+\frac{1}{2}}\left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2}+\frac{j\omega_c\Delta t}{8}}\right)|_k\tilde{E}_y|_{k+\frac{1}{2}}^{n+\frac{1}{2}} \\
& +\left(1+\left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2}+\frac{j\omega_c\Delta t}{8}}\right)|_k\left(\left(\frac{p_{11}\Delta t}{4\mu_0\Delta z}\right)|_{k-\frac{1}{2}}+\left(\frac{p_{11}\Delta t}{4\mu_0\Delta z}\right)|_{k+\frac{1}{2}}\right)\right)\tilde{E}_y|_k^{n+\frac{1}{2}} \\
& =\hat{e}_y|_k^n+\left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2}+\frac{j\omega_c\Delta t}{8}}\right)|_k(\hat{h}_x|_{k+\frac{1}{2}}^n-\hat{h}_x|_{k-\frac{1}{2}}^n),
\end{aligned} \tag{4.43}$$

with tridiagonal matrix coefficient. This equation can be obtained by substituting the RHS of implicit update equation for $\tilde{H}_x|_{k+\frac{1}{2}}^{n+\frac{1}{2}}$ in (4.30) into the update equation for $\tilde{E}_y|_k^{n+\frac{1}{2}}$ in (4.29). Notice that (4.43) has few and simple RHS terms, which is a feature of the efficient ADI splitting formulae [26]. This makes the proposed method easy and efficient to implement. Upon the update of $\tilde{E}_y|_k^{n+\frac{1}{2}}$, the remaining fields can be determined explicitly with

$$\tilde{H}_x|_{k+\frac{1}{2}}^{n+\frac{1}{2}}=\hat{h}_x|_{k+\frac{1}{2}}^n+\left(\frac{p_{11}\Delta t}{4\mu_0\Delta z}\right)|_{k+\frac{1}{2}}(\tilde{E}_y|_{k+1}^{n+\frac{1}{2}}-\tilde{E}_y|_k^{n+\frac{1}{2}}) \tag{4.44}$$

$$\tilde{H}_y|_{k+\frac{1}{2}}^{n+\frac{1}{2}}=\hat{h}_y|_{k+\frac{1}{2}}^n+\left(\frac{p_{21}\Delta t}{4\mu_0\Delta z}\right)|_{k+\frac{1}{2}}(\tilde{E}_y|_{k+1}^{n+\frac{1}{2}}-\tilde{E}_y|_k^{n+\frac{1}{2}}) \tag{4.45}$$

$$\tilde{M}_x|_{k+\frac{1}{2}}^{n+\frac{1}{2}}=\hat{m}_x|_{k+\frac{1}{2}}^n+\left(\frac{p_{31}\Delta t}{4\mu_0\Delta z}\right)|_{k+\frac{1}{2}}(\tilde{E}_y|_{k+1}^{n+\frac{1}{2}}-\tilde{E}_y|_k^{n+\frac{1}{2}}) \tag{4.46}$$

$$\tilde{M}_y|_{k+\frac{1}{2}}^{n+\frac{1}{2}}=\hat{m}_y|_{k+\frac{1}{2}}^n+\left(\frac{p_{41}\Delta t}{4\mu_0\Delta z}\right)|_{k+\frac{1}{2}}(\tilde{E}_y|_{k+1}^{n+\frac{1}{2}}-\tilde{E}_y|_k^{n+\frac{1}{2}}) \tag{4.47}$$

$$\tilde{E}_x|_k^{n+\frac{1}{2}}=\hat{e}_x|_k^n+\left(\frac{\frac{\kappa_{xy}\Delta t}{4\Delta z}}{\frac{1}{2}+\frac{j\omega_c\Delta t}{8}}\right)|_k(\tilde{H}_x|_{k+\frac{1}{2}}^{n+\frac{1}{2}}-\tilde{H}_x|_{k-\frac{1}{2}}^{n+\frac{1}{2}}). \tag{4.48}$$

A similar set of update procedure can be deduced for Substep 2 to complete the update of $\tilde{\mathbf{u}}^{n+1}$.

4.2.2 Without Magnetic Media

(a) With Gain

In this section, we present the CE-ADI-FDTD formulation for modeling inhomogeneous media with anisotropic permittivity tensor and gain. The presented formulation will be especially useful in analyzing lasing properties of materials such as laser dye doped cholesteric liquid crystals, as will be discussed in Section 4.3.2. We assume an active medium that has an anisotropic inverse permittivity tensor $\bar{\bar{\kappa}}$, in which, elements κ_{xz} , κ_{zx} , κ_{yz} and κ_{zy} equal to zero. To model the active part of the medium, we adopt the four-level atomic system approach, as presented in [121], with an energy band structure depicted in Fig. 4.1. The electron carriers are all initially at ground state N_0 . With electrical pumping P_r , some electrons are excited to the higher energy level of N_3 . Due to thermal decay, some electrons drop back to lower energy levels of N_2 (and back to N_0 from N_1). Transitions between N_1 and N_2 levels result in gain or absorption. The rate equations governing the changes in carrier distributions at each level are

$$\frac{dN_0(z,t)}{dt} = \frac{N_1(z,t)}{\tau_{10}} - P_r N_0(z,t) \quad (4.49)$$

$$\frac{dN_1(z,t)}{dt} = -\frac{1}{\hbar\omega_a} \mathbf{E}(z,t) \cdot \frac{d\mathbf{P}(z,t)}{dt} + \frac{N_2(z,t)}{\tau_{21}} - \frac{N_1(z,t)}{\tau_{10}} \quad (4.50)$$

$$\frac{dN_2(z,t)}{dt} = +\frac{1}{\hbar\omega_a} \mathbf{E}(z,t) \cdot \frac{d\mathbf{P}(z,t)}{dt} + \frac{N_3(z,t)}{\tau_{32}} - \frac{N_2(z,t)}{\tau_{21}} \quad (4.51)$$

$$\frac{dN_3(z,t)}{dt} = -\frac{N_3(z,t)}{\tau_{32}} + P_r N_0(z,t). \quad (4.52)$$

In (4.50) and (4.51), the terms $\frac{1}{\hbar\omega_a} \mathbf{E}(z,t) \cdot \frac{d\mathbf{P}(z,t)}{dt}$ and $\frac{N_2(z,t)}{\tau_{21}}$ correspond to gain/absorption and spontaneous emission, respectively.

The interactions between the electromagnetic field and the active media can macroscopically be described as dipole oscillations between respective energy levels. For the

Figure 4.1: Energy band structure of four-level atomic system.

case here, the dipole oscillation between N_1 and N_2 levels is denoted by the polarization density term $\mathbf{P}$ whose evolution is governed by a 'Harmonic Oscillator' equation of motion as

$$\frac{\partial^2 \mathbf{P}}{\partial t^2} + \gamma_a \frac{\partial \mathbf{P}}{\partial t} + \omega_a^2 \mathbf{P} = \alpha_a \mathbf{E}. \quad (4.53)$$

In (4.53), $\alpha_a = \frac{\gamma_r e^2}{\gamma_c m} \Delta N(z, t)$, γ_a is the full width at half-maximum linewidth of the atomic transition and ω_a is the central frequency of the oscillation. In (4.53), we note that $\mathbf{P}$ is not only driven by the external field $\mathbf{E}$ but also by the difference between the microscopic electron carrier concentrations ΔN at energy levels 1 and 2 as $\Delta N(z, t) = N_1(z, t) - N_2(z, t)$. Under population inversion condition ($N_2(z, t) > N_1(z, t)$), gain is achieved. The pumping should be sufficiently large enough to attain this condition. The net field that is the sum of the original $\mathbf{E}$ field and the contribution due to the dipole oscillations $\mathbf{P}$ is then expressed in Maxwell's magnetic curl equation as

$$\frac{\partial \mathbf{E}}{\partial t} = \bar{\mathbf{k}} \nabla \times \mathbf{H} - \bar{\mathbf{k}} \frac{\partial \mathbf{P}}{\partial t}. \quad (4.54)$$

The electric curl equation is expressed as

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E}. \quad (4.55)$$

Equations (4.53)-(4.55) and the carrier rate equations (4.49)-(4.52) form a self-consistent set of equations that govern the spatial and temporal behaviour of fields in an active medium with anisotropic permittivity tensor.

To obtain a CE-ADI formulation for fields in active medium, we first express the set of equations (4.53)-(4.55) in first-order system form (similar approach was taken for magnetic media in Section 4.2.1). To do so, we utilize the substitution

$$\frac{\partial \mathbf{P}}{\partial t} = \mathbf{Q} \quad (4.56)$$

and reduce (4.53) to

$$\frac{\partial \mathbf{Q}}{\partial t} + \gamma_a \mathbf{Q} + \omega_a^2 \mathbf{P} = \alpha_a \mathbf{E}. \quad (4.57)$$

Now, assuming propagation along z -direction, equations (4.56)-(4.57) and (4.54)-(4.55) can be expressed in first-order system form as

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{M} \mathbf{u}.$$

Upon using the relation $\mathbf{u} = \Re \{ \tilde{\mathbf{u}} e^{j\omega_c t} \}$, the first-order system form for CE fields can be attained as

$$\frac{\partial \tilde{\mathbf{u}}}{\partial t} = (-j\omega_c \mathbf{I} + \mathbf{M}) \tilde{\mathbf{u}}, \quad (4.58)$$

in which field envelope vector $\tilde{\mathbf{u}}$ is

$$\tilde{\mathbf{u}} = \begin{bmatrix} \tilde{E}_x & \tilde{E}_y & \tilde{H}_x & \tilde{H}_y & \tilde{P}_x & \tilde{Q}_x & \tilde{P}_y & \tilde{Q}_y \end{bmatrix}^T, \quad (4.59)$$

ω_c is the carrier angular-frequency, $\mathbf{I}$ is the identity matrix and matrix $\mathbf{M}$ is

$$\mathbf{M} = \begin{bmatrix} 0 & 0 & \kappa_{xy} \frac{\partial}{\partial z} & -\kappa_{xx} \frac{\partial}{\partial z} & 0 & -\kappa_{xx} & 0 & -\kappa_{xy} \\ 0 & 0 & \kappa_{yy} \frac{\partial}{\partial z} & -\kappa_{yx} \frac{\partial}{\partial z} & 0 & -\kappa_{yx} & 0 & -\kappa_{yy} \\ 0 & \frac{1}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \alpha_a & 0 & 0 & 0 & -\omega_a^2 & -\gamma_a & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \alpha_a & 0 & 0 & 0 & 0 & -\omega_a^2 & -\gamma_a \end{bmatrix}. \quad (4.60)$$

The system matrix $(-j\omega_c \mathbf{I} + \mathbf{M})$ is next split into two sub-matrices $\mathbf{A}^n$ and $\mathbf{B}^n$ as

$$\mathbf{A}^n = \begin{bmatrix} -\frac{j\omega_c}{2} & 0 & \kappa_{xy} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & -\kappa_{xy} \\ 0 & -\frac{j\omega_c}{2} & \kappa_{yy} \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & -\kappa_{yy} \\ 0 & \frac{1}{\mu_0} \frac{\partial}{\partial z} & -\frac{j\omega_c}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{j\omega_c}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{j\omega_c}{2} & \frac{1}{2} & 0 & 0 \\ \frac{\alpha_a^n}{2} & 0 & 0 & 0 & -\frac{\omega_a^2}{2} & \frac{-j\omega_c - \gamma_a}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{j\omega_c}{2} & \frac{1}{2} \\ 0 & \frac{\alpha_a^n}{2} & 0 & 0 & 0 & 0 & -\frac{\omega_a^2}{2} & \frac{-j\omega_c - \gamma_a}{2} \end{bmatrix} \quad (4.61)$$

$$\mathbf{B}^n = \begin{bmatrix} -\frac{j\omega_c}{2} & 0 & 0 & -\kappa_{xx} \frac{\partial}{\partial z} & 0 & -\kappa_{xx} & 0 & 0 \\ 0 & -\frac{j\omega_c}{2} & 0 & -\kappa_{yx} \frac{\partial}{\partial z} & 0 & -\kappa_{yx} & 0 & 0 \\ 0 & 0 & -\frac{j\omega_c}{2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{\mu_0} \frac{\partial}{\partial z} & 0 & 0 & -\frac{j\omega_c}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{j\omega_c}{2} & \frac{1}{2} & 0 & 0 \\ \frac{\alpha_a^n}{2} & 0 & 0 & 0 & -\frac{\omega_a^2}{2} & \frac{-j\omega_c - \gamma_a}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{j\omega_c}{2} & \frac{1}{2} \\ 0 & \frac{\alpha_a^n}{2} & 0 & 0 & 0 & 0 & -\frac{\omega_a^2}{2} & \frac{-j\omega_c - \gamma_a}{2} \end{bmatrix}. \quad (4.62)$$

Note that the carrier distributions in α_a are sampled at the n th time step, which is the reason for the superscript n appearing in $\mathbf{A}^n$ and $\mathbf{B}^n$. The differential operators $\frac{\partial}{\partial z}$ and $-\frac{\partial}{\partial z}$ are split into $\mathbf{A}^n$ and $\mathbf{B}^n$, respectively. In the magnetic curl equations, the elements of $\tilde{Q}_\xi$ (for $\xi = x, y$) are split into the same matrices as the associated differential operators. The association is made by looking at elements of $\tilde{Q}_\xi$ and differential operators having the same inverse permittivity tensor element. The elements corresponding to the auxiliary differential equations (4.56)-(4.57) are split equally into $\mathbf{A}^n$ and $\mathbf{B}^n$, as noted by the factors of half in the respective elements in $\mathbf{A}^n$ and $\mathbf{B}^n$.

The sub-matrices $\mathbf{A}^n$ and $\mathbf{B}^n$ are next used in the conventional ADI splitting formulae, in place of the time-independent $\mathbf{A}$ and $\mathbf{B}$, as

$$(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A}^n) \tilde{\mathbf{u}}^{n+\frac{1}{2}} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{B}^n) \tilde{\mathbf{u}}^n \quad (4.63)$$

$$(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B}^n) \tilde{\mathbf{u}}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{A}^n) \tilde{\mathbf{u}}^{n+\frac{1}{2}}. \quad (4.64)$$

In [26], an efficient ADI splitting formulae with matrix-operator-free right-hand sides was deduced from the conventional ADI splitting formulae, for time-independent sub-

matrices. This efficient ADI splitting formulae is presented in (4.7)-(4.10). We next modify the efficient ADI splitting formulae to accomodate time-dependent sub-matrices.

We first introduce an auxiliary vector $\tilde{\mathbf{v}}$ with elements

$$\tilde{\mathbf{v}} = \begin{bmatrix} \tilde{e}_x & \tilde{e}_y & \tilde{h}_x & \tilde{h}_y & \tilde{p}_x & \tilde{q}_x & \tilde{p}_y & \tilde{q}_y \end{bmatrix}^T. \quad (4.65)$$

We next equate the right-hand sides of (4.63) and (4.64) to

$$\tilde{\mathbf{v}}^n = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{B}^n) \tilde{\mathbf{u}}^n \quad (4.66)$$

$$\tilde{\mathbf{v}}^{n+\frac{1}{2}} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{A}^n) \tilde{\mathbf{u}}^{n+\frac{1}{2}}, \quad (4.67)$$

respectively. Now the update equation for $\tilde{\mathbf{v}}^n$ can be deduced as

$$\tilde{\mathbf{v}}^n = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{B}^n) \tilde{\mathbf{u}}^n \quad (4.68)$$

$$\begin{aligned} &= 2\tilde{\mathbf{u}}^n - (\mathbf{I} - \frac{\Delta t}{2} \mathbf{B}^n) \tilde{\mathbf{u}}^n \\ &= 2\tilde{\mathbf{u}}^n - (\mathbf{I} - \frac{\Delta t}{2} \mathbf{B}^{n-1}) \tilde{\mathbf{u}}^n - \frac{\Delta t}{2} (\mathbf{B}^{n-1} - \mathbf{B}^n) \tilde{\mathbf{u}}^n \\ &= 2\tilde{\mathbf{u}}^n - (\mathbf{I} + \frac{\Delta t}{2} \mathbf{A}^{n-1}) \tilde{\mathbf{u}}^{n-\frac{1}{2}} - \frac{\Delta t}{2} (\mathbf{B}^{n-1} - \mathbf{B}^n) \tilde{\mathbf{u}}^n \\ &= 2\tilde{\mathbf{u}}^n - \tilde{\mathbf{v}}^{n-\frac{1}{2}} - \frac{\Delta t}{2} (\mathbf{B}^{n-1} - \mathbf{B}^n) \tilde{\mathbf{u}}^n \\ &= (2\mathbf{I} - \frac{\Delta t}{2} (\mathbf{B}^{n-1} - \mathbf{B}^n)) \tilde{\mathbf{u}}^n - \tilde{\mathbf{v}}^{n-\frac{1}{2}}. \end{aligned} \quad (4.69)$$

Similarly, the update equation for $\tilde{\mathbf{v}}^{n+\frac{1}{2}}$ can be deduced as

$$\tilde{\mathbf{v}}^{n+\frac{1}{2}} = (\mathbf{I} + \frac{\Delta t}{2} \mathbf{A}^n) \tilde{\mathbf{u}}^{n+\frac{1}{2}} \quad (4.70)$$

$$\begin{aligned} &= 2\tilde{\mathbf{u}}^{n+\frac{1}{2}} - (\mathbf{I} - \frac{\Delta t}{2} \mathbf{A}^n) \tilde{\mathbf{u}}^{n+\frac{1}{2}} \\ &= 2\tilde{\mathbf{u}}^{n+\frac{1}{2}} - (\mathbf{I} + \frac{\Delta t}{2} \mathbf{B}^n) \tilde{\mathbf{u}}^n \\ &= 2\tilde{\mathbf{u}}^{n+\frac{1}{2}} - \tilde{\mathbf{v}}^n. \end{aligned} \quad (4.71)$$

When $\mathbf{B}^{n-1} = \mathbf{B}^n$, the matrix operations on the right-hand side of (4.68) and (4.70) are both replaced by simpler vector arithmetic operations in (4.69) and (4.71), respectively. The efficient ADI splitting formulae that is modified for time-dependent matrices can thus be written in compact form as

$$\text{Substep 1 : } \tilde{\mathbf{v}}^n = (\mathbf{I} - \frac{\Delta t}{4}(\mathbf{B}^{n-1} - \mathbf{B}^n))\tilde{\mathbf{u}}^n - \tilde{\mathbf{v}}^{n-\frac{1}{2}} \quad (4.72)$$

$$(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{A}^n)\tilde{\mathbf{u}}^{n+\frac{1}{2}} = \tilde{\mathbf{v}}^n \quad (4.73)$$

$$\text{Substep 2 : } \tilde{\mathbf{v}}^{n+\frac{1}{2}} = \tilde{\mathbf{u}}^{n+\frac{1}{2}} - \tilde{\mathbf{v}}^n \quad (4.74)$$

$$(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{B}^n)\tilde{\mathbf{u}}^{n+1} = \tilde{\mathbf{v}}^{n+\frac{1}{2}}. \quad (4.75)$$

Note that we have scaled (4.72)-(4.75) by a factor of half and set $\frac{1}{2}\tilde{\mathbf{v}}^n$ to $\tilde{\mathbf{v}}^n$ and $\frac{1}{2}\tilde{\mathbf{v}}^{n+\frac{1}{2}}$ to $\tilde{\mathbf{v}}^{n+\frac{1}{2}}$.

To obtain simpler update equations, we further introduce a matrix $\mathbf{G}$

$$\mathbf{G} = \begin{bmatrix} \frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\frac{1}{2} + \frac{\Delta t(\gamma_a + j\omega_c)}{8}}{Det} & \frac{\frac{\Delta t}{8}}{Det} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{-\frac{\omega_a^2 \Delta t}{8}}{Det} & \frac{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}{Det} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\frac{1}{2} + \frac{\Delta t(\gamma_a + j\omega_c)}{8}}{Det} & \frac{\frac{\Delta t}{8}}{Det} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{-\frac{\omega_a^2 \Delta t}{8}}{Det} & \frac{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}{Det} \end{bmatrix} \quad (4.76)$$

in which

$$Det = \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8}\right) \left(\frac{1}{2} + \frac{(\gamma_a + j\omega_c) \Delta t}{8}\right) + \frac{(\omega_a \Delta t)^2}{64} \quad (4.77)$$

and multiply it throughout (4.72)-(4.75). This scales the diagonal part of the matrices $(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{A}^n)$ and $(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{B}^n)$ in (4.73) and (4.75), respectively, to 1. We then set $\mathbf{G}\tilde{\mathbf{v}}^n = \hat{\mathbf{v}}^n$ and $\mathbf{G}\tilde{\mathbf{v}}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^{n+\frac{1}{2}}$. The efficient ADI splitting formulae for time-dependent matrices is arrived at in its final compact form as

$$\text{Substep 1 : } \hat{\mathbf{v}}^n = \mathbf{G}(\mathbf{I} - \frac{\Delta t}{4}(\mathbf{B}^{n-1} - \mathbf{B}^n))\tilde{\mathbf{u}}^n - \hat{\mathbf{v}}^{n-\frac{1}{2}} \quad (4.78)$$

$$(\mathbf{I} - \frac{\Delta t}{4}\hat{\mathbf{A}}^n)\tilde{\mathbf{u}}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^n \quad (4.79)$$

$$\text{Substep 2 : } \hat{\mathbf{v}}^{n+\frac{1}{2}} = \mathbf{G}\tilde{\mathbf{u}}^{n+\frac{1}{2}} - \hat{\mathbf{v}}^n \quad (4.80)$$

$$(\mathbf{I} - \frac{\Delta t}{4}\hat{\mathbf{B}}^n)\tilde{\mathbf{u}}^{n+1} = \hat{\mathbf{v}}^{n+\frac{1}{2}}. \quad (4.81)$$

in which, the scaled $\hat{\mathbf{A}}^n$ and $\hat{\mathbf{B}}^n$ are

$$\hat{\mathbf{A}}^n = \begin{bmatrix} 0 & 0 & \frac{\kappa_{xy} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 & \frac{-\kappa_{xy}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \\ 0 & 0 & \frac{\kappa_{yy} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 & \frac{-\kappa_{yy}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \\ 0 & \frac{\frac{1}{\mu_0} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_a^n \Delta t}{Det 16} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_a^n}{Det} \frac{1}{2} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8}\right) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\alpha_a^n \Delta t}{Det 16} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\alpha_a^n}{Det} \frac{1}{2} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8}\right) & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.82)$$

$$\hat{\mathbf{B}}^n = \begin{bmatrix} 0 & 0 & 0 & -\frac{\kappa_{xx} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & \frac{-\kappa_{xx}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\kappa_{yx} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & \frac{-\kappa_{yx}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\frac{1}{\mu_0} \frac{\partial}{\partial z}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_a^n}{Det} \frac{\Delta t}{16} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\alpha_a^n}{Det} \frac{1}{2} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8} \right) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\alpha_a^n}{Det} \frac{\Delta t}{16} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\alpha_a^n}{Det} \frac{1}{2} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8} \right) & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

(4.83)

Upon expansion of (4.78)-(4.81), the following set of update equations can be attained:

Substep 1

Auxiliary updating of $\hat{\mathbf{v}}^n$ in (4.78):

$$\hat{e}_x|^n = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{E}_x|^n - \hat{e}_x|^{n-\frac{1}{2}} \quad (4.84)$$

$$\hat{e}_y|^n = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{E}_y|^n - \hat{e}_y|^{n-\frac{1}{2}} \quad (4.85)$$

$$\hat{h}_x|^n = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{H}_x|^n - \hat{h}_x|^{n-\frac{1}{2}} \quad (4.86)$$

$$\hat{h}_y|^n = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{H}_y|^n - \hat{h}_y|^{n-\frac{1}{2}} \quad (4.87)$$

$$\hat{p}_x|^n = \frac{\frac{1}{2} + \frac{\Delta t}{8}(\gamma_a + j\omega_c)}{Det} \tilde{P}_x|^n + \frac{\frac{\Delta t}{8}}{Det} \tilde{Q}_x|^n + \frac{\frac{\Delta t^2}{64}}{Det} (\alpha_a^n - \alpha_a^{n-1}) \tilde{E}_x|^n - \hat{p}_x|^{n-\frac{1}{2}} \quad (4.88)$$

$$\hat{q}_x|^n = -\frac{\frac{\omega_a^2 \Delta t}{8}}{Det} \tilde{P}_x|^n + \frac{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}{Det} \tilde{Q}_x|^n + \frac{\frac{\Delta t}{8}}{Det} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8} \right) (\alpha_a^n - \alpha_a^{n-1}) \tilde{E}_x|^n - \hat{q}_x|^{n-\frac{1}{2}} \quad (4.89)$$

$$\hat{p}_y|^n = \frac{\frac{1}{2} + \frac{\Delta t}{8}(\gamma_a + j\omega_c)}{Det} \tilde{P}_y|^n + \frac{\frac{\Delta t}{8}}{Det} \tilde{Q}_y|^n + \frac{\frac{\Delta t^2}{64}}{Det} (\alpha_a^n - \alpha_a^{n-1}) \tilde{E}_y|^n - \hat{p}_y|^{n-\frac{1}{2}} \quad (4.90)$$

$$\hat{q}_y|^n = -\frac{\frac{\omega_a^2 \Delta t}{8}}{Det} \tilde{P}_y|^n + \frac{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}{Det} \tilde{Q}_y|^n + \frac{\frac{\Delta t}{8}}{Det} \left(\frac{1}{2} + \frac{j\omega_c \Delta t}{8} \right) (\alpha_a^n - \alpha_a^{n-1}) \tilde{E}_y|^n - \hat{q}_y|^{n-\frac{1}{2}} \quad (4.91)$$

Intermediate updating of $\tilde{\mathbf{u}}^{n+\frac{1}{2}}$ in (4.79):

$$\tilde{E}_x|^{n+\frac{1}{2}} = \hat{e}_x|^n + \left(\frac{\frac{\kappa_{xy} \Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \frac{\partial \tilde{H}_x|^{n+\frac{1}{2}}}{\partial z} - \left(\frac{\frac{\kappa_{xy} \Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{Q}_y|^{n+\frac{1}{2}} \quad (4.92)$$

$$\tilde{E}_y|^{n+\frac{1}{2}} = \hat{e}_y|^n + \left(\frac{\frac{\kappa_{yy} \Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \frac{\partial \tilde{H}_x|^{n+\frac{1}{2}}}{\partial z} - \left(\frac{\frac{\kappa_{yy} \Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{Q}_y|^{n+\frac{1}{2}} \quad (4.93)$$

$$\tilde{H}_x|^{n+\frac{1}{2}} = \hat{h}_x|^n + \left(\frac{\frac{\Delta t}{4\mu_0}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \frac{\partial \tilde{E}_y|^{n+\frac{1}{2}}}{\partial z} \quad (4.94)$$

$$\tilde{H}_y|^{n+\frac{1}{2}} = \hat{h}_y|^n \quad (4.95)$$

$$\tilde{P}_x|^{n+\frac{1}{2}} = \hat{p}_x|^n + \frac{\alpha_a^n \frac{\Delta t^2}{64}}{Det} \tilde{E}_x|^{n+\frac{1}{2}} \quad (4.96)$$

$$\tilde{Q}_x|^{n+\frac{1}{2}} = \hat{q}_x|^n + \frac{\alpha_a^n \frac{\Delta t}{8} (\frac{1}{2} + \frac{j\omega_c \Delta t}{8})}{Det} \tilde{E}_x|^{n+\frac{1}{2}} \quad (4.97)$$

$$\tilde{P}_y|^{n+\frac{1}{2}} = \hat{p}_y|^n + \frac{\alpha_a^n \frac{\Delta t^2}{64}}{Det} \tilde{E}_y|^{n+\frac{1}{2}} \quad (4.98)$$

$$\tilde{Q}_y|^{n+\frac{1}{2}} = \hat{q}_y|^n + \frac{\alpha_a^n \frac{\Delta t}{8} (\frac{1}{2} + \frac{j\omega_c \Delta t}{8})}{Det} \tilde{E}_y|^{n+\frac{1}{2}} \quad (4.99)$$

Substep 2

Auxiliary updating of $\hat{\mathbf{v}}^{n+\frac{1}{2}}$ in (4.80):

$$\hat{e}_x|^{n+\frac{1}{2}} = (\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}) \tilde{E}_x|^{n+\frac{1}{2}} - \hat{e}_x|^n \quad (4.100)$$

$$\hat{e}_y|^{n+\frac{1}{2}} = (\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}) \tilde{E}_y|^{n+\frac{1}{2}} - \hat{e}_y|^n \quad (4.101)$$

$$\hat{h}_x|^{n+\frac{1}{2}} = (\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}) \tilde{H}_x|^{n+\frac{1}{2}} - \hat{h}_x|^n \quad (4.102)$$

$$\hat{h}_y|^{n+\frac{1}{2}} = (\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}) \tilde{H}_y|^{n+\frac{1}{2}} - \hat{h}_y|^n \quad (4.103)$$

$$\hat{p}_x|^{n+\frac{1}{2}} = \frac{\frac{1}{2} + \frac{\Delta t}{8} (\gamma_a + j\omega_c)}{Det} \tilde{P}_x|^{n+\frac{1}{2}} + \frac{\frac{\Delta t}{8}}{Det} \tilde{Q}_x|^{n+\frac{1}{2}} - \hat{p}_x|^n \quad (4.104)$$

$$\hat{q}_x|^{n+\frac{1}{2}} = -\frac{\frac{\omega_a^2 \Delta t}{8}}{Det} \tilde{P}_x|^{n+\frac{1}{2}} + \frac{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}{Det} \tilde{Q}_x|^{n+\frac{1}{2}} - \hat{q}_x|^n \quad (4.105)$$

$$\hat{p}_y|^{n+\frac{1}{2}} = \frac{\frac{1}{2} + \frac{\Delta t}{8} (\gamma_a + j\omega_c)}{Det} \tilde{P}_y|^{n+\frac{1}{2}} + \frac{\frac{\Delta t}{8}}{Det} \tilde{Q}_y|^{n+\frac{1}{2}} - \hat{p}_y|^n \quad (4.106)$$

$$\hat{q}_y|^{n+\frac{1}{2}} = -\frac{\frac{\omega_a^2 \Delta t}{8}}{Det} \tilde{P}_y|^{n+\frac{1}{2}} + \frac{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}{Det} \tilde{Q}_y|^{n+\frac{1}{2}} - \hat{q}_y|^n \quad (4.107)$$

Final updating of $\tilde{\mathbf{u}}^{n+1}$ in (4.81):

$$\tilde{E}_x|^{n+1} = \hat{e}_x|^{n+\frac{1}{2}} - \left(\frac{\frac{\kappa_{xx}\Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right) \frac{\partial \tilde{H}_y|^{n+1}}{\partial z} - \left(\frac{\frac{\kappa_{yx}\Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right) \tilde{Q}_x|^{n+1} \quad (4.108)$$

$$\tilde{E}_y|^{n+1} = \hat{e}_y|^{n+\frac{1}{2}} - \left(\frac{\frac{\kappa_{yx}\Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right) \frac{\partial \tilde{H}_y|^{n+1}}{\partial z} - \left(\frac{\frac{\kappa_{xx}\Delta t}{4}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right) \tilde{Q}_x|^{n+1} \quad (4.109)$$

$$\tilde{H}_x|^{n+1} = \hat{h}_x|^{n+\frac{1}{2}} \quad (4.110)$$

$$\tilde{H}_y|^{n+1} = \hat{h}_y|^{n+\frac{1}{2}} - \left(\frac{\frac{\Delta t}{4\mu_0}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right) \frac{\partial \tilde{E}_x|^{n+1}}{\partial z} \quad (4.111)$$

$$\tilde{P}_x|^{n+1} = \hat{p}_x|^{n+\frac{1}{2}} + \frac{\alpha_a^n \frac{\Delta t^2}{64}}{Det} \tilde{E}_x|^{n+1} \quad (4.112)$$

$$\tilde{Q}_x|^{n+1} = \hat{q}_x|^{n+\frac{1}{2}} + \frac{\alpha_a^n \frac{\Delta t}{8} \left(\frac{1}{2} + \frac{j\omega_c\Delta t}{8}\right)}{Det} \tilde{E}_x|^{n+1} \quad (4.113)$$

$$\tilde{P}_y|^{n+1} = \hat{p}_y|^{n+\frac{1}{2}} + \frac{\alpha_a^n \frac{\Delta t^2}{64}}{Det} \tilde{E}_y|^{n+1} \quad (4.114)$$

$$\tilde{Q}_y|^{n+1} = \hat{q}_y|^{n+\frac{1}{2}} + \frac{\alpha_a^n \frac{\Delta t}{8} \left(\frac{1}{2} + \frac{j\omega_c\Delta t}{8}\right)}{Det} \tilde{E}_y|^{n+1} \quad (4.115)$$

The actual numerical update of components of $\tilde{\mathbf{u}}$ is next discussed. For spatial discretization we assume grid cells of size Δz with staggered $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{H}}$ and collocated $\tilde{\mathbf{E}}, \tilde{\mathbf{P}}$ and $\tilde{\mathbf{Q}}$ field positions. To cater for inhomogeneity in media, update coefficients are explicitly sampled at either k or $k + \frac{1}{2}$ positions (denoted as subscripts), which correspond to $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{H}}$ field positions, respectively. At the beginning of every time step, carrier distributions are first updated at every spatial point in which active medium is present. The update is performed via a discrete form of the carrier rate equations (4.49)-(4.52),

as follows:

$$N_0^n = N_0^{n-1} + \Delta t \left(\frac{N_1^{n-1}}{\tau_{10}} - P_r^{n-1} N_0^{n-1} \right) \quad (4.116)$$

$$N_1^n = N_1^{n-1} + \Delta t \left(-\frac{1}{\hbar\omega_a} \mathbf{E}^{n-1} \cdot \mathbf{Q}^{n-1} + \frac{N_2^{n-1}}{\tau_{21}} - \frac{N_1^{n-1}}{\tau_{10}} \right) \quad (4.117)$$

$$N_2^n = N_2^{n-1} + \Delta t \left(\frac{1}{\hbar\omega_a} \mathbf{E}^{n-1} \cdot \mathbf{Q}^{n-1} + \frac{N_3^{n-1}}{\tau_{32}} - \frac{N_2^{n-1}}{\tau_{21}} \right) \quad (4.118)$$

$$N_3^n = N_3^{n-1} + \Delta t \left(-\frac{N_3^{n-1}}{\tau_{32}} + P_r^{n-1} N_0^{n-1} \right). \quad (4.119)$$

Once the carriers have been updated, the coefficient α_a^n that has a term $N_1^n - N_2^n$ can be determined.

Next, we begin the field update using the CE-ADI formulation. Substep 1 is first performed, in which, the update of auxiliary fields $\hat{\mathbf{v}}^n$ is first directly computed using explicit update equations (4.84)-(4.91). Next, the intermediate fields $\tilde{\mathbf{u}}^{n+\frac{1}{2}}$ are updated using (4.92)-(4.99). In this part, the implicit update of $\tilde{E}_y|_k^{n+\frac{1}{2}}$ is first performed from a system of linear equations in the form

$$\begin{aligned} & - \left(\frac{\frac{\Delta t}{4\mu_0\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_{k-\frac{1}{2}} \left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_k \tilde{E}_y|_{k-1}^{n+\frac{1}{2}} - \left(\frac{\frac{\Delta t}{4\mu_0\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_{k+\frac{1}{2}} \left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_k \tilde{E}_y|_{k+1}^{n+\frac{1}{2}} \\ & + \left(1 + \left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_k \left(\left(\frac{\frac{\Delta t}{4\mu_0\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_{k-\frac{1}{2}} + \left(\frac{\frac{\Delta t}{4\mu_0\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_{k+\frac{1}{2}} \right) + \frac{\Delta t^2 \kappa_{yy}}{32} \frac{\alpha_a^n}{Det} \right) \tilde{E}_y|_k^{n+\frac{1}{2}} \\ & = \hat{e}_y|_k^n + \left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_k (\hat{h}_x|_{k+\frac{1}{2}}^n - \hat{h}_x|_{k-\frac{1}{2}}^n) - \left(\frac{\frac{\kappa_{yy}\Delta t}{4\Delta z}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) |_k \hat{q}_y|_k^n, \end{aligned} \quad (4.120)$$

with tridiagonal matrix. Note that a significant difference between this tridiagonal equation for active medium and the tridiagonal equation for passive medium (for example (4.43)) is the presence of a left-hand side term $\frac{\Delta t^2 \kappa_{yy}}{32} \frac{\alpha_a^n}{Det}$ that is time-dependent. Hence, unlike passive medium case (where left-hand side information can be precomputed before simulation starts), the left-hand side information for active medium case requires

updating at every time step, just after α_a^n has been determined. Equation (4.120) can be obtained by substituting the RHS of implicit update equation for $\tilde{H}_x|_{k+\frac{1}{2}}^{n+\frac{1}{2}}$ and $\tilde{Q}_y|_k^{n+\frac{1}{2}}$ in (4.94) and (4.99), respectively, into the update equation for $\tilde{E}_y|_k^{n+\frac{1}{2}}$ in (4.93). Upon the update of $\tilde{E}_y|_k^{n+\frac{1}{2}}$, the remaining fields can be determined explicitly. A similar set of update procedure can be deduced for Substep 2 to complete the update of $\tilde{\mathbf{u}}^{n+1}$.

(b) Without Gain

For nonmagnetic (no ferrite) periodic structures without gain materials, a more efficient form of the CE-ADI-FDTD method can be attained compared to the conventional form presented in [64]. The efficient CE-ADI-FDTD formulation can be determined from (4.18)-(4.21) by setting the ferrite parameters to zero and removing fields $\tilde{M}_x$ and $\tilde{M}_y$. After some manipulations, the following efficient CE-ADI-FDTD method can be deduced for field advancement over both substeps 1 and 2:

Substep 1

Auxiliary updating of $\hat{e}_y|_k^n, \hat{h}_x|_k^n$:

$$\hat{e}_y|_k^n = \hat{\alpha}|_k(\tilde{E}_y|_k^{n-\frac{1}{2}} - \hat{e}_y|_k^{n-1}) + \frac{\beta^{yx}|_k}{\beta^{xx}|_k}(\tilde{E}_x|_k^n - \alpha|_k\hat{e}_x|_k^{n-\frac{1}{2}}) \quad (4.121)$$

$$\hat{h}_x|_{k+\frac{1}{2}}^n = \hat{\alpha}|_{k+\frac{1}{2}}^2 \hat{h}_x|_{k+\frac{1}{2}}^{n-1} + \delta|_{k+\frac{1}{2}}(\tilde{E}_y|_{k+1}^{n-\frac{1}{2}} - \tilde{E}_y|_k^{n-\frac{1}{2}}) \quad (4.122)$$

Intermediate updating of $\tilde{E}_y|_k^{n+\frac{1}{2}}$ via tridiagonal matrix solution:

$$\begin{aligned} & -\frac{\gamma|_{k-\frac{1}{2}}\beta^{yy}|_k}{\alpha|_k}\tilde{E}_y|_{k-1}^{n+\frac{1}{2}} + \frac{1 + \gamma|_{k-\frac{1}{2}}\beta^{yy}|_k + \gamma|_{k+\frac{1}{2}}\beta^{yy}|_k}{\alpha|_k}\tilde{E}_y|_k^{n+\frac{1}{2}} - \frac{\gamma|_{k+\frac{1}{2}}\beta^{yy}|_k}{\alpha|_k}\tilde{E}_y|_{k+1}^{n+\frac{1}{2}} \\ & = \hat{e}_y|_k^n + \frac{\beta^{yy}|_k}{\alpha|_k}(\hat{h}_x|_{k+\frac{1}{2}}^n - \hat{h}_x|_{k-\frac{1}{2}}^n) \end{aligned} \quad (4.123)$$

Substep 2

Auxiliary updating of $\hat{e}_x|^{n+\frac{1}{2}}, \hat{h}_y|^{n+\frac{1}{2}}$:

$$\hat{e}_x|_k^{n+\frac{1}{2}} = \hat{\alpha}|_k(\tilde{E}_x|_k^n - \hat{e}_x|_k^{n-\frac{1}{2}}) + \frac{\beta^{xy}|_k}{\beta^{yy}|_k}(\tilde{E}_y|_k^{n+\frac{1}{2}} - \alpha|_k \hat{e}_y|_k^n) \quad (4.124)$$

$$\hat{h}_y|_{k+\frac{1}{2}}^{n+\frac{1}{2}} = \hat{\alpha}|_{k+\frac{1}{2}}^2 \hat{h}_y|_{k+\frac{1}{2}}^{n-\frac{1}{2}} - \delta|_{k+\frac{1}{2}}(\tilde{E}_x|_{k+1}^n - \tilde{E}_x|_k^n) \quad (4.125)$$

Final updating of $\tilde{E}_x|^{n+1}$ via tridiagonal matrix solution:

$$\begin{aligned} & -\frac{\gamma|_{k-\frac{1}{2}}\beta^{xx}|_k}{\alpha|_k}\tilde{E}_x|_{k-1}^{n+1} + \frac{1 + \gamma|_{k-\frac{1}{2}}\beta^{xx}|_k + \gamma|_{k+\frac{1}{2}}\beta^{xx}|_k}{\alpha|_k}\tilde{E}_x|_k^{n+1} - \frac{\gamma|_{k+\frac{1}{2}}\beta^{xx}|_k}{\alpha|_k}\tilde{E}_x|_{k+1}^{n+1} \\ & = \hat{e}_x|_k^{n+\frac{1}{2}} - \frac{\beta^{xx}|_k}{\alpha|_k}(\hat{h}_y|_{k+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{h}_y|_{k-\frac{1}{2}}^{n+\frac{1}{2}}) \end{aligned} \quad (4.126)$$

with the update coefficients

$$\begin{aligned} \alpha|_k &= \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right)|_k, & \hat{\alpha}|_k &= \alpha|_k - 1, & \gamma|_k &= \left(\frac{\Delta t\alpha}{4\mu_0\Delta z}\right)|_k \\ \delta|_k &= (\alpha\hat{\alpha}\gamma)|_k, & \beta^\xi|_k &= \left(\frac{\Delta t\alpha\kappa_\xi}{4\Delta z}\right)|_k. \end{aligned}$$

The remaining envelope fields at $n+1$ time step can be output from the updated fields in (4.121)-(4.126) as

$$\tilde{E}_y|_k^{n+1} = \alpha|_k(\tilde{E}_y|_k^{n+\frac{1}{2}} - \hat{e}_y|_k^n) + \frac{\beta^{yx}|_k}{\beta^{xx}|_k}(\tilde{E}_x|_k^{n+1} - \alpha|_k \hat{e}_x|_k^{n+\frac{1}{2}}) \quad (4.127)$$

$$\tilde{H}_x|_{k+\frac{1}{2}}^{n+1} = \hat{\alpha}|_{k+\frac{1}{2}}\hat{h}_x|_{k+\frac{1}{2}}^n + \gamma|_{k+\frac{1}{2}}\alpha|_{k+\frac{1}{2}}(\tilde{E}_y|_{k+1}^{n+\frac{1}{2}} - \tilde{E}_y|_k^{n+\frac{1}{2}}) \quad (4.128)$$

$$\tilde{H}_y|_{k+\frac{1}{2}}^{n+1} = \hat{h}_y|_{k+\frac{1}{2}}^{n+\frac{1}{2}} - \gamma|_{k+\frac{1}{2}}(\tilde{E}_x|_{k+1}^{n+1} - \tilde{E}_x|_k^{n+1}). \quad (4.129)$$

Note that the final $\tilde{E}_y|_k^{n+1}$, $\tilde{H}_x|_{k+\frac{1}{2}}^{n+1}$ and $\tilde{H}_y|_{k+\frac{1}{2}}^{n+1}$ fields need not be computed during field advancement and can instead be output with (4.127)-(4.129), only when required.

Using (4.121)-(4.126), field advancement can be performed in a more concise and efficient manner with simpler and fewer RHS terms compared to the conventional CE-

Table 4.1: Flops count and number of RHS terms comparison between proposed efficient and conventional CE-ADI-FDTD methods

Method		Conventional [64]	Proposed Efficient
Auxiliary	M/D	0	10
	A/S	0	10
Implicit	M/D	12	2
	A/S	10	4
Explicit	M/D	20	0
	A/S	16	0
Total	M/D	32	12
	A/S	26	14
RHS terms		70	32

ADI-FDTD method proposed in [64]. The use of auxiliary updating in the fundamental ADI splitting formulae [26] aids this reduction in RHS terms. To compare the computational efficiency in detail, Table 4.1 lists the floating point operations (flops) count including number of multiplications/divisions (M/D) and additions/subtractions (A/S) and number of RHS terms including number of field and coefficient variables, required for one complete time step. The flops count and number of RHS terms are attained from the RHSs of the proposed method and compared with that of [64]. From the table, it is observed that the total flops count (M/D+A/S) and number of RHS terms reduce from 58 to 26 and 70 to 32, respectively, in the proposed method.

4.2.3 An Extension to Two-Dimensional Case

In the previous Sections (4.2.1)-(4.2.2), formulations were primarily presented for the case of 1-D wave propagation along the z direction. In this section, we present an extension of the CE-ADI-FDTD method for case of 2-D wave propagation in anisotropic media. We consider the TM_z wave propagation case with a saturated ferrite biased in the z direction. The permeability of the medium is thus represented by a tensor with

anisotropy in the xy plane. The governing Maxwell's equations for this 2-D problem are

$$\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \frac{\partial H_y}{\partial x} - \frac{1}{\epsilon} \frac{\partial H_x}{\partial y} \quad (4.130)$$

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_z}{\partial y} - \frac{\partial M_x}{\partial t} \quad (4.131)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_z}{\partial x} - \frac{\partial M_y}{\partial t} \quad (4.132)$$

$$\frac{\partial M_x}{\partial t} = \omega_m H_y - \omega_0 M_y - \alpha \frac{\partial M_y}{\partial t} \quad (4.133)$$

$$\frac{\partial M_y}{\partial t} = -\omega_m H_x + \omega_0 M_x + \alpha \frac{\partial M_x}{\partial t}. \quad (4.134)$$

In (4.133)-(4.134), M_x and M_y are components of magnetization vector $\mathbf{M}$ and $\omega_m = \gamma \mu_0 M_s$ and $\omega_0 = \gamma \mu_0 H_0$. M_s and H_0 denote the magnitudes of saturation magnetization and dc biasing magnetic field, respectively, and γ is the gyromagnetic ratio with α being the ferrite loss constant.

Much similar to the approach presented in Sections (4.2.1)-(4.2.2), the complex-envelope fields of (4.130)-(4.134) are first expressed in a first-order system form as

$$\frac{\partial \tilde{\mathbf{u}}}{\partial t} = (-j\omega_c \mathbf{I} + \mathbf{M}) \tilde{\mathbf{u}} \quad (4.135)$$

in which field envelope vector $\tilde{\mathbf{u}}$ is

$$\tilde{\mathbf{u}} = \begin{bmatrix} \tilde{E}_z & \tilde{H}_x & \tilde{H}_y & \tilde{M}_x & \tilde{M}_y \end{bmatrix}^T, \quad (4.136)$$

ω_c is the carrier angular-frequency, $\mathbf{I}$ is the identity matrix and matrix $\mathbf{M}$ is

$$\mathbf{M} = \begin{bmatrix} 0 & -\frac{1}{\varepsilon} \frac{\partial}{\partial y} & \frac{1}{\varepsilon} \frac{\partial}{\partial x} & 0 & 0 \\ -\frac{1}{\mu_0} \frac{\partial}{\partial y} & -\frac{\omega_m \alpha}{\alpha^2 + 1} & -\frac{\omega_m}{\alpha^2 + 1} & \frac{\omega_0 \alpha}{\alpha^2 + 1} & \frac{\omega_0}{\alpha^2 + 1} \\ \frac{1}{\mu_0} \frac{\partial}{\partial x} & \frac{\omega_m}{\alpha^2 + 1} & -\frac{\omega_m \alpha}{\alpha^2 + 1} & -\frac{\omega_0}{\alpha^2 + 1} & \frac{\omega_0 \alpha}{\alpha^2 + 1} \\ 0 & \frac{\omega_m \alpha}{\alpha^2 + 1} & \frac{\omega_m}{\alpha^2 + 1} & -\frac{\omega_0 \alpha}{\alpha^2 + 1} & -\frac{\omega_0}{\alpha^2 + 1} \\ 0 & -\frac{\omega_m}{\alpha^2 + 1} & \frac{\omega_m \alpha}{\alpha^2 + 1} & \frac{\omega_0}{\alpha^2 + 1} & -\frac{\omega_0 \alpha}{\alpha^2 + 1} \end{bmatrix} \quad (4.137)$$

The system matrix $(-j\omega_c \mathbf{I} + \mathbf{M})$ is next split into two sub-matrices $\mathbf{A}$ and $\mathbf{B}$ as

$$\mathbf{A} = \begin{bmatrix} -\frac{j\omega_c}{2} & 0 & \frac{1}{\varepsilon} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & -\xi_1 & -\xi_2 & \xi_3 & \xi_4 \\ \frac{1}{\mu_0} \frac{\partial}{\partial x} & \xi_2 & -\xi_1 & -\xi_4 & \xi_3 \\ 0 & \xi_5 & \xi_2 & -\xi_6 & -\xi_4 \\ 0 & -\xi_2 & \xi_5 & \xi_4 & -\xi_6 \end{bmatrix} \quad (4.138)$$

$$\mathbf{B} = \begin{bmatrix} -\frac{j\omega_c}{2} & -\frac{1}{\varepsilon} \frac{\partial}{\partial y} & 0 & 0 & 0 \\ -\frac{1}{\mu_0} \frac{\partial}{\partial y} & -\xi_1 & -\xi_2 & \xi_3 & \xi_4 \\ 0 & \xi_2 & -\xi_1 & -\xi_4 & \xi_3 \\ 0 & \xi_5 & \xi_2 & -\xi_6 & -\xi_4 \\ 0 & -\xi_2 & \xi_5 & \xi_4 & -\xi_6 \end{bmatrix}. \quad (4.139)$$

The elements ξ in matrices $\mathbf{A}$ and $\mathbf{B}$ are

$$\begin{aligned} \xi_1 &= \frac{j\omega_c}{2} + \frac{\omega_m \alpha}{2(\alpha^2 + 1)} & \xi_2 &= \frac{\omega_m}{2(\alpha^2 + 1)} & \xi_3 &= \frac{\omega_0 \alpha}{2(\alpha^2 + 1)} \\ \xi_6 &= \frac{j\omega_c}{2} + \frac{\omega_0 \alpha}{2(\alpha^2 + 1)} & \xi_4 &= \frac{\omega_0}{2(\alpha^2 + 1)} & \xi_5 &= \frac{\omega_m \alpha}{2(\alpha^2 + 1)}. \end{aligned}$$

The matrices $\mathbf{A}$ and $\mathbf{B}$ are next used in the efficient ADI splitting formulae and following similar steps in Section (4.2.1), that diagonalize the left-hand side matrices, the proposed CE-ADI-FDTD method can be written as

$$\text{Substep 1 : } \hat{\mathbf{v}}^n = \mathbf{G}\tilde{\mathbf{u}}^n - \hat{\mathbf{v}}^{n-\frac{1}{2}} \quad (4.140)$$

$$\left(\mathbf{I} - \frac{\Delta t}{4}\hat{\mathbf{A}}\right)\tilde{\mathbf{u}}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^n \quad (4.141)$$

$$\text{Substep 2 : } \hat{\mathbf{v}}^{n+\frac{1}{2}} = \mathbf{G}\tilde{\mathbf{u}}^{n+\frac{1}{2}} - \hat{\mathbf{v}}^n \quad (4.142)$$

$$\left(\mathbf{I} - \frac{\Delta t}{4}\hat{\mathbf{B}}\right)\tilde{\mathbf{u}}^{n+1} = \hat{\mathbf{v}}^{n+\frac{1}{2}} \quad (4.143)$$

where the vectors $\mathbf{G}\tilde{\mathbf{v}}$ have been grouped by an auxiliary vector $\hat{\mathbf{v}} = \mathbf{G}\tilde{\mathbf{v}}$ that is denoted as

$$\hat{\mathbf{v}} = \begin{bmatrix} \hat{e}_z & \hat{h}_x & \hat{h}_y & \hat{m}_x & \hat{m}_y \end{bmatrix}^T. \quad (4.144)$$

In (4.140) and (4.142), $\mathbf{G}$ is written as

$$\mathbf{G} = \begin{bmatrix} \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}}\right)\mathbf{I}_{(1 \times 1)} & \mathbf{0}_{(1 \times 4)} \\ \mathbf{0}_{(4 \times 1)} & \mathbf{P}_{(4 \times 4)} \end{bmatrix}$$

with

$$\mathbf{P} = \begin{bmatrix} \frac{1}{2} + \frac{\Delta t \xi_1}{4} & \frac{\Delta t \xi_2}{4} & -\frac{\Delta t \xi_3}{4} & -\frac{\Delta t \xi_4}{4} \\ -\frac{\Delta t \xi_2}{4} & \frac{1}{2} + \frac{\Delta t \xi_1}{4} & \frac{\Delta t \xi_4}{4} & -\frac{\Delta t \xi_3}{4} \\ -\frac{\Delta t \xi_5}{4} & -\frac{\Delta t \xi_2}{4} & \frac{1}{2} + \frac{\Delta t \xi_6}{4} & \frac{\Delta t \xi_4}{4} \\ \frac{\Delta t \xi_2}{4} & -\frac{\Delta t \xi_5}{4} & -\frac{\Delta t \xi_4}{4} & \frac{1}{2} + \frac{\Delta t \xi_6}{4} \end{bmatrix}^{-1},$$

while in (4.141) and (4.143), $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ are expressed as

$$\hat{\mathbf{A}} = \begin{bmatrix} 0 & 0 & \frac{\frac{1}{\epsilon} \frac{\partial}{\partial x}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 \\ \frac{p_{12}}{\mu_0} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ \frac{p_{22}}{\mu_0} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ \frac{p_{32}}{\mu_0} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ \frac{p_{42}}{\mu_0} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\hat{\mathbf{B}} = \begin{bmatrix} 0 & -\frac{\frac{1}{\epsilon} \frac{\partial}{\partial y}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} & 0 & 0 & 0 \\ -\frac{p_{11}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 \\ -\frac{p_{21}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 \\ -\frac{p_{31}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 \\ -\frac{p_{41}}{\mu_0} \frac{\partial}{\partial y} & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Upon expansion of (4.140)-(4.143), the following set of update equations can be attained:

Substep 1

Auxiliary updating of $\hat{\mathbf{v}}^n$ in (4.140):

$$\hat{e}_z|^n = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \tilde{E}_z|^n - \hat{e}_z|^{n-\frac{1}{2}} \quad (4.145)$$

$$\begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^n = \mathbf{P} \begin{bmatrix} \tilde{H}_x \\ \tilde{H}_y \\ \tilde{M}_x \\ \tilde{M}_y \end{bmatrix}^n - \begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^{n-\frac{1}{2}} \quad (4.146)$$

Intermediate updating of $\tilde{\mathbf{u}}^{n+\frac{1}{2}}$ in (4.141):

$$\tilde{E}_z|^{n+\frac{1}{2}} = \hat{e}_z|^n + \left(\frac{\frac{\Delta t}{4\epsilon}}{\frac{1}{2} + \frac{j\omega_c \Delta t}{8}} \right) \frac{\partial \tilde{H}_y|^{n+\frac{1}{2}}}{\partial x} \quad (4.147)$$

$$\tilde{H}_x|^{n+\frac{1}{2}} = \hat{h}_x|^n + \left(\frac{p_{12}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_z|^{n+\frac{1}{2}}}{\partial x} \quad (4.148)$$

$$\tilde{H}_y|^{n+\frac{1}{2}} = \hat{h}_y|^n + \left(\frac{p_{22}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_z|^{n+\frac{1}{2}}}{\partial x} \quad (4.149)$$

$$\tilde{M}_x|^{n+\frac{1}{2}} = \hat{m}_x|^n + \left(\frac{p_{32}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_z|^{n+\frac{1}{2}}}{\partial x} \quad (4.150)$$

$$\tilde{M}_y|^{n+\frac{1}{2}} = \hat{m}_y|^n + \left(\frac{p_{42}\Delta t}{4\mu_0} \right) \frac{\partial \tilde{E}_z|^{n+\frac{1}{2}}}{\partial x} \quad (4.151)$$

Substep 2

Auxiliary updating of $\hat{\mathbf{v}}^{n+\frac{1}{2}}$ in (4.142):

$$\hat{e}_z|^{n+\frac{1}{2}} = \left(\frac{1}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right) \tilde{E}_z|^{n+\frac{1}{2}} - \hat{e}_z|^n \quad (4.152)$$

$$\begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^{n+\frac{1}{2}} = \mathbf{P} \begin{bmatrix} \tilde{H}_x \\ \tilde{H}_y \\ \tilde{M}_x \\ \tilde{M}_y \end{bmatrix}^{n+\frac{1}{2}} - \begin{bmatrix} \hat{h}_x \\ \hat{h}_y \\ \hat{m}_x \\ \hat{m}_y \end{bmatrix}^n \quad (4.153)$$

Final updating of $\tilde{\mathbf{u}}^{n+1}$ in (4.143):

$$\tilde{E}_z|^{n+1} = \hat{e}_z|^{n+\frac{1}{2}} - \left(\frac{\frac{\Delta t}{4\epsilon}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}}\right) \frac{\partial \tilde{H}_x|^{n+1}}{\partial y} \quad (4.154)$$

$$\tilde{H}_x|^{n+1} = \hat{h}_x|^{n+\frac{1}{2}} - \left(\frac{p_{11}\Delta t}{4\mu_0}\right) \frac{\partial \tilde{E}_z|^{n+1}}{\partial y} \quad (4.155)$$

$$\tilde{H}_y|^{n+1} = \hat{h}_y|^{n+\frac{1}{2}} - \left(\frac{p_{21}\Delta t}{4\mu_0}\right) \frac{\partial \tilde{E}_z|^{n+1}}{\partial y} \quad (4.156)$$

$$\tilde{M}_x|^{n+1} = \hat{m}_x|^{n+\frac{1}{2}} - \left(\frac{p_{31}\Delta t}{4\mu_0}\right) \frac{\partial \tilde{E}_z|^{n+1}}{\partial y} \quad (4.157)$$

$$\tilde{M}_y|^{n+1} = \hat{m}_y|^{n+\frac{1}{2}} - \left(\frac{p_{41}\Delta t}{4\mu_0}\right) \frac{\partial \tilde{E}_z|^{n+1}}{\partial y} \quad (4.158)$$

The actual numerical update of components of $\tilde{\mathbf{u}}$ is next discussed. For spatial discretization, we assume grid cells of size Δx and Δy with staggered $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{H}}$ and collocated $\tilde{\mathbf{H}}$ and $\tilde{\mathbf{M}}$ field positions. To cater for inhomogeneity in media, update coefficients are explicitly sampled at (i, j) , $(i, j + \frac{1}{2})$ or $(i + \frac{1}{2}, j)$ positions (denoted as subscripts), which correspond to $\tilde{E}_z$, $\tilde{H}_x$ and $\tilde{H}_y$ field positions, respectively. Consider the Substep 1 as an illustration. First, the update of auxiliary fields $\hat{\mathbf{v}}^n$ is directly determined using explicit update equations (4.145)-(4.146). Next, the update of intermediate fields $\tilde{\mathbf{u}}^{n+\frac{1}{2}}$ is performed using (4.147)-(4.151). In this part, the implicit update of $\tilde{E}_z|_{i,j}^{n+\frac{1}{2}}$ is first

attained from a system of linear equations in the form

$$\begin{aligned}
& - \left(\frac{p_{22}\Delta t}{4\mu_0\Delta z} \right) \Big|_{i-\frac{1}{2},j} \left(\frac{\frac{\Delta t}{4\epsilon\Delta x}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) \Big|_{i,j} \tilde{E}_z|_{i-1,j}^{n+\frac{1}{2}} - \left(\frac{p_{22}\Delta t}{4\mu_0\Delta z} \right) \Big|_{i+\frac{1}{2},j} \left(\frac{\frac{\Delta t}{4\epsilon\Delta x}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) \Big|_{i,j} \tilde{E}_z|_{i+1,j}^{n+\frac{1}{2}} \\
& + \left(1 + \left(\frac{\frac{\Delta t}{4\epsilon\Delta x}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) \Big|_{i,j} \left(\left(\frac{p_{22}\Delta t}{4\mu_0\Delta x} \right) \Big|_{i-\frac{1}{2},j} + \left(\frac{p_{22}\Delta t}{4\mu_0\Delta x} \right) \Big|_{i+\frac{1}{2},j} \right) \right) \tilde{E}_z|_{i,j}^{n+\frac{1}{2}} \\
& = \hat{e}_z|_{i,j}^n + \left(\frac{\frac{\Delta t}{4\epsilon\Delta x}}{\frac{1}{2} + \frac{j\omega_c\Delta t}{8}} \right) \Big|_{i,j} (\hat{h}_y|_{i+\frac{1}{2},j}^n - \hat{h}_y|_{i-\frac{1}{2},j}^n),
\end{aligned} \tag{4.159}$$

with tridiagonal matrix coefficient. This equation can be obtained by substituting the RHS of implicit update equation for $\tilde{H}_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$ in (4.149) into the update equation for $\tilde{E}_z|_{i,j}^{n+\frac{1}{2}}$ in (4.147). Upon the update of $\tilde{E}_z|_{i,j}^{n+\frac{1}{2}}$, the remaining fields can be determined explicitly with

$$\tilde{H}_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \hat{h}_y|_{i+\frac{1}{2},j}^n + \left(\frac{p_{22}\Delta t}{4\mu_0\Delta x} \right) \Big|_{i+\frac{1}{2},j} (\tilde{E}_z|_{i+1,j}^{n+\frac{1}{2}} - \tilde{E}_z|_{i,j}^{n+\frac{1}{2}}) \tag{4.160}$$

$$\tilde{M}_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \hat{m}_y|_{i+\frac{1}{2},j}^n + \left(\frac{p_{42}\Delta t}{4\mu_0\Delta x} \right) \Big|_{i+\frac{1}{2},j} (\tilde{E}_z|_{i+1,j}^{n+\frac{1}{2}} - \tilde{E}_z|_{i,j}^{n+\frac{1}{2}}) \tag{4.161}$$

$$\tilde{H}_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \hat{h}_x|_{i,j+\frac{1}{2}}^n + \left(\frac{p_{12}}{p_{22}} \right) \Big|_{i,j+\frac{1}{2}} (\tilde{H}_y|_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{h}_y|_{i+\frac{1}{2}}^{n+\frac{1}{2}})_{i,j+\frac{1}{2}} \tag{4.162}$$

$$\tilde{M}_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \hat{m}_x|_{i,j+\frac{1}{2}}^n + \left(\frac{p_{32}}{p_{22}} \right) \Big|_{i,j+\frac{1}{2}} (\tilde{H}_y|_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{h}_y|_{i+\frac{1}{2}}^{n+\frac{1}{2}})_{i,j+\frac{1}{2}}. \tag{4.163}$$

Note that (4.162) and (4.163) can be attained by substituting $\frac{\partial \tilde{E}_z|_{i,j}^{n+\frac{1}{2}}}{\partial x}$ in (4.149) into (4.148) and (4.150), respectively. To compute $\tilde{H}_x$ and $\tilde{M}_x$, $\tilde{H}_y$ and $\hat{h}_y$ have to be interpolated from neighboring four points to $(i, j + \frac{1}{2})$, since they are explicitly sampled at $(i + \frac{1}{2}, j)$. This interpolation can be performed using

$$\tilde{H}_y|_{i,j+\frac{1}{2}} = \frac{1}{4} (\tilde{H}_y|_{i+\frac{1}{2},j} + \tilde{H}_y|_{i-\frac{1}{2},j} + \tilde{H}_y|_{i+\frac{1}{2},j+1} + \tilde{H}_y|_{i-\frac{1}{2},j+1}). \tag{4.164}$$

A similar set of update procedure can be deduced for Substep 2 to complete the update of $\tilde{\mathbf{u}}^{n+1}$.

4.3 Numerical Results

4.3.1 Experiment 1: Magnetic Photonic Crystal

Figure 4.2: $N = 16$ periodically stacked array with each unit cell composed of one ferrite layer F and two misaligned anisotropic dielectric layers $A1$ and $A2$.

In this section, we demonstrate the proposed CE-ADI-FDTD method for efficient modeling of lossy magnetic PhC. Consider a $N = 16$ periodically stacked array with unit cells, each composed of one ferrite layer F and two misaligned anisotropic dielectric layers $A1$ and $A2$ (layer sequence of F - $A2$ - $A1$ towards $+z$ direction). Fig. 4.2 illustrates this stacked array. A similar array is presented in [45]. Layers $A1$ and $A2$ are characterized by free space permeability and the following permittivity tensor with $\epsilon_{A1} = \epsilon_{A2} = 31.39$, $\delta_{A1} = \delta_{A2} = 13.61$, $\phi_{A1} = 0^\circ$ and $\phi_{A2} = 45^\circ$:

$$\bar{\bar{\epsilon}} = \epsilon_0 \begin{bmatrix} \epsilon_A + \delta_A \cos(2\phi_A) & \delta_A \sin(2\phi_A) & 0 \\ \delta_A \sin(2\phi_A) & \epsilon_A - \delta_A \cos(2\phi_A) & 0 \\ 0 & 0 & \epsilon_{zz} \end{bmatrix}. \quad (4.165)$$

Figure 4.3: (a) Band diagram and (b) transmittance plots for lossless magnetic PhC. L is the thickness of a unit cell, $L = L_F + L_{A2} + L_{A1}$. Unit of frequency is Hz.

Layer F is characterized by scalar permittivity of $14.5\epsilon_0$ and ferrite parameters of $\omega_m = 3.5441 \times 10^{10}$ rad/s and $\omega_0 = 9.4178 \times 10^{10}$ rad/s. For a lossy ferrite case, $\alpha = 0.01$. The layer thicknesses are $L_{A1} = L_{A2} = 1$ mm and $L_F = 0.25$ mm.

The band diagram and transmittance of the lossless ($\alpha = 0$) magnetic PhC is next analyzed using the transfer matrix method. The band diagram is first analyzed from Fig. 4.3(a). The diagram highlights a spectral asymmetry in the region of 10.65 GHz, where a stationary inflection point (SIP) occurs for wave propagation in the $+z$ direction and no SIP occurs for wave propagation in the corresponding $-z$ direction. At the SIP frequency region, electromagnetic wave propagates in the $+z$ direction with vanishing group velocity ($\frac{\partial\omega}{\partial k} \rightarrow 0$) and an increase in wave amplitude [105], [110]. However, electromagnetic wave propagates in the $-z$ direction as a normal wave. This different propagation behaviours for opposite directions illustrates a non-reciprocity in the magnetic PhC.

Figure 4.4: (a) Band diagram and (b) transmittance plots for lossless *nonmagnetic* PhC. Ferrite layer F of magnetic PhC is simply replaced by a free space layer. Unit of frequency is Hz.

The transmittance of a $N = 16$ lossless magnetic PhC is next analyzed in Fig. 4.3(b) specifically for two cases; one in which the incident field is towards the $+z$ direction (direction of SIP) and another in which the incident field is towards the $-z$ direction. The polarization of incident fields in the $+z$ and $-z$ directions are selected as $\phi = 32.5^\circ$ and $\phi = 0^\circ$, respectively, as indicated in Fig. 4.2. This correspond to maximum transmittances of 0.99 and 0.75 in the $+z$ and $-z$ directions, respectively, at 10.65 GHz (SIP frequency region). These different transmittances for opposite directions further illustrate the non-reciprocal behaviour of the magnetic PhC [106]. To further appreciate this, we also considered the case when the ferrite layer F is simply replaced by a free space layer. In this case, a *nonmagnetic* PhC is attained with spectral symmetry in its band diagram (split-band edges [107]), as shown in Fig. 4.4(a). This ought to indicate a reciprocal behaviour of the PhC. Indeed, this reciprocity is further illustrated in the transmittance plot in Fig. 4.4(b), where identical transmittances of 0.99 is observed for both $+z$ and $-z$ directed incident fields.

The proposed CE-ADI-FDTD method is next used to efficiently compute the time-average field intensity $|\mathbf{E}|^2$ inside the magnetic PhC. The simulations are performed

Figure 4.5: Normalized $|\mathbf{E}|^2$ versus position for (a) lossless and (b) lossy ferrite cases. Markers $\circ$, $+$ and $\square$ attained with proposed CE-ADI-FDTD method at CFLN of 100, 150 and 200 respectively. Continuous line plot attained with explicit FDTD method at CFLN of 1.

with uniform cell size of $\Delta z = 0.01\text{mm}$, time step size of $\Delta t = \text{CFLN} \frac{0.98\Delta z}{c}$ and 10 PML layers with quartic conductivity profile. For excitation, a $+z$ directed continuous wave with electric field of unit amplitude, polarization $\phi = 32.5^\circ$ and carrier frequency $\omega_c \approx 6.6901 \times 10^{10}\text{rad/s}$ is used. Fig. 4.5 plots the normalized $|\mathbf{E}|^2$ (normalized to the incident $|\mathbf{E}|^2$) using the proposed CE-ADI-FDTD method at different CFLN values and for both lossless and lossy ferrite cases. Plotted together for comparison, is the normalized $|\mathbf{E}|^2$ using the explicit FDTD method presented in [45]. For both the lossless and lossy cases, good agreement is shown between the proposed CE-ADI-FDTD method at various CFLN values and the explicit FDTD method. However, the CPU times consumed by the proposed CE-ADI-FDTD method at CFLN=100, 150 and 200 are 24.4%, 15.3% and 11.5% of the CPU time consumed by the explicit FDTD method, respectively. The proposed method thus consumes much less computational time while maintaining good agreement with the explicit FDTD method.

Figure 4.6: Normalized $|\mathbf{E}|^2$ versus position for (a) lossless and (b) lossy ferrite cases, using proposed CE-ADI-FDTD method at CFLN=200. Continuous and dotted line plots indicate incident field excitation towards the $+z$ and $-z$ directions, respectively.

To further appreciate the non-reciprocity in the magnetic PhC, the time-average field intensity $|\mathbf{E}|^2$ is compared for the cases of incident fields excited towards the $+z$ and $-z$ directions. The incident field polarizations are $\phi = 32.5^\circ$ and $\phi = 0^\circ$ for propagations towards $+z$ and $-z$ directions, respectively. The proposed CE-ADI-FDTD method with CFLN=200 is used to compute the corresponding $|\mathbf{E}|^2$. Fig. 4.6 plots the normalized $|\mathbf{E}|^2$ for cases of incident fields excited towards the $+z$ and $-z$ directions and for both lossless and lossy ferrite cases. For lossless case, the figure shows that a larger field amplitude (maximum 3.435) is attained for $+z$ excitation as compared to the $-z$ excitation (maximum 2.044). The larger amplitude for $+z$ excitation is due to the SIP mode being $+z$ directed. Note however that for $-z$ excitation, the SIP mode is *partially* excited due to multiple boundary reflections in the finite sized PhC [106]. A similar observation can be made for the lossy case.

4.3.2 Experiment 2: Nonmagnetic Photonic Crystal

(a) With Gain

In this section, we demonstrate the proposed efficient CE-ADI-FDTD method for modeling an anisotropic periodic structure with gain. An example of such a structure is a cholesteric liquid crystal (CLC) with laser doped dye [120]-[121]. Under conditions of chirality, CLCs can have rodlike molecular structure that vary in direction in a particular plane over a particular direction. For the case considered here, the CLCs have structural variance in the xy plane over the z direction, as illustrated in Fig. 4.7. This physical variation, that is periodic over the z direction, is taken into account by an anisotropic permittivity tensor as

$$\bar{\bar{\epsilon}}(z) = \epsilon_0 \begin{bmatrix} \epsilon_o + \Delta\epsilon \sin^2 \theta(z) & \Delta\epsilon \sin \theta(z) \cos \theta(z) & 0 \\ \Delta\epsilon \sin \theta(z) \cos \theta(z) & \epsilon_o + \Delta\epsilon \cos^2 \theta(z) & 0 \\ 0 & 0 & \epsilon_o \end{bmatrix}, \quad (4.166)$$

in which, ϵ_o and ϵ_e ($\Delta\epsilon = \epsilon_e - \epsilon_o$) are the ordinary and extraordinary dielectric constants of the anisotropic medium, respectively, and $\theta(z)$ is the angle between the optical axis and the y axis. $\theta(z)$ varies along the z direction. When doped with laser dye, low-threshold lasing can be observed at the edge of the stop band, where a high density of states exists [120].

A similar experiment to [121] is considered here where the CLC with gain is sandwiched between glass substrates, that is terminated by PML absorbing boundary conditions, as shown in Fig. 4.7. The dielectric tensor of CLC has elements of $\epsilon_o = 1.5^2$ and $\epsilon_e = 1.7^2$ with a helical pitch of 400nm, hence $\theta(z) = \frac{2\pi z}{400nm}$. The glass substrate has effective permittivity of 1.5^2 . The lengths of CLC and glass substrate are 20um and

Figure 4.7: Simulation of cholesteric liquid crystal (CLC) with gain.

5um, respectively. The laser dye has the following specifications: central wavelength $\lambda_a = 600nm$ and $\omega_a = \frac{2\pi c}{\lambda_a}$, $\gamma_a = 9.1744 \times 10^{13}$, $\gamma_r = \frac{1}{\tau_{21}}$ and $\gamma_c = \frac{e^2}{m} \frac{\omega_a^2}{6\pi\epsilon_0 c^3}$ where e , m and c are the electron charge, electron mass and speed of light in vacuum, respectively. The transition times are $\tau_{32} = 10^{-13}s$, $\tau_{21} = 10^{-9}s$ and $\tau_{10} = 10^{-11}s$. The total electron density is $5.5 \times 6.02 \times 10^{23}$. Initially, all electrons are at ground state N_0 .

The CE-ADI-FDTD simulation uses a uniform cell size of $\Delta z = 1 \times 10^{-8}m$ and time step size of $\Delta t = \Delta t_{CFL} CFLN$, in which, $\Delta t_{CFL} = 2 \times 10^{-17}s$ and CFLN is the Courant number (conventional FDTD has CFLN=1). 15 PML layers with quartic conductivity profile are used to truncate the simulation. The pumping rate P_r is set to $10^{10}s^{-1}$. Note that the largest time step size for conventional explicit FDTD is on the order of 10^{-17} whereas the largest transition time for active medium is on the order of 10^{-9} . Judging from these numbers, it can be anticipated that large number of iterations is required for the system to evolve to steady-state. Hence, this motivates the use of CE-ADI-FDTD that can allow for larger time step sizes as compared to conventional FDTD, thereby reducing the number of iterations.

Figure 4.8: Time-domain plot of electric fields E_x and E_y sampled at observation point in glass substrate.

In the first part of the experiment, we excite the CLC layer with a weak and short Gaussian pulse seed at centre wavelength $\lambda_c = 600\text{nm}$. At an observation point in the right-most glass substrate, the electric fields E_x and E_y are attained using the CE-ADI-FDTD at CFLN=5. Hence, the number of iterations is 5 times lesser than conventional FDTD. Fig. 4.8 plots these fields in time-domain. The figure shows that after about 4ps, steady-state oscillations of fields with very large amplitudes on the order of 10^6 are being produced. This is likely due to lasing emissions. On closer inspection of steady state E_x and E_y fields at around 5ps in Fig. 4.9, it can be seen that the fields are delayed with respect to each other by about 0.5fs. This translates to a phase shift of $\frac{\pi}{2}$ and thus the lasing emission is circularly polarized, as was also shown in [121]. The verified circular polarization can be attributed to the helical structure of the CLC cavity [121].

In the second part of the experiment, the transmittance is attained by first launching a Gaussian pulse from one side of the CLC with no gain, recording the fields at the other end of the CLC and then taking their Fourier transforms. Fig. 4.10 plots the transmittance along with the lasing spectrum from the electric fields. A stop band can be observed centred at 640nm. Just at the left-most edge of the stop band, a sharp lasing

Figure 4.9: Steady-state time-domain plot of electric fields E_x and E_y around the time of 5ps.

Figure 4.10: Plot of transmittance and lasing spectrum.

peak occurs at 600nm. This verifies the band edge lasing as was similarly illustrated in [121]. The proposed CE-ADI-FDTD method is thus verified to be able to simulate anisotropic periodic structures with gain media while requiring fewer iterations compared to the conventional explicit FDTD method.

(b) Without Gain

In this section, we demonstrate the proposed efficient CE-ADI-FDTD method for modeling of a nonmagnetic PhC with split band edges (SBE) on its band diagram and without gain. Consider a periodically stacked array with $N = 11$ unit cells. Each cell is composed of two anisotropic layers $A1$ and $A2$ that are characterized by the permittivity tensor (4.165) and a single isotropic layer B that is assumed to be free space (layer sequence of $A1$ - B - $A2$ towards $+z$ direction). A SBE dispersion relation can be realized in each unit cell by configuring its A layer material parameters as $\epsilon_{A1} = \epsilon_{A2} = 13.61$, $\delta_{A1} = \delta_{A2} = 12.4$, $\phi_{A1} = 0^\circ$ and $\phi_{A2} = 35^\circ$ and the layer thicknesses as $L_{A1} = L_{A2} = 0.270545\text{m}$ and $L_B = 0.45891\text{m}$ [65].

Figs. 4.11(a)-(b) plot the transmittance and band diagram of such a SBE PhC, respectively. In Fig. 4.11(a), unit transmittance is observed at the Fabry-Perot resonance $\omega \approx 3.1441034 \times 10^8 \text{rad/s}$, independent of incident wave polarization [107]. From the symmetric band diagram, it can be deduced that this frequency corresponds to two reciprocal propagating modes operating close to the split band edges with vanishing group velocity. The significance of having two reciprocal pairs of propagating modes is that the incident wave radiation can be fully coupled to the SBE PhC regardless of incident polarization [65], [107]. This is illustrated as well in Fig. 4.11(a).

The time-averaged field intensity $|\mathbf{E}|^2$ inside the SBE PhC with $N = 11$ is next determined using the proposed efficient CE-ADI-FDTD method and compared with the method in [64]. The following simulation parameters are used: $\Delta z_{A1} = \Delta z_{A2} = 2.505\text{mm}$ and $\Delta z_B = 2.494\text{mm}$, $\Delta t = \text{CFLN} \frac{\Delta z_B}{c_0}$, 10 PML boundary layers with quartic polynomial conductivity profile and a unit amplitude continuous wave source with carrier frequency $\omega \approx 3.1441034 \times 10^8 \text{rad/s}$. Fig. 4.12 plots the field intensity $|\mathbf{E}|^2$ using the proposed

Figure 4.11: (a) Transmittance for different incident wave polarizations ϕ_{pol} and (b) band diagram illustrating the split band edges of a SBE PhC with $N = 11$. ϕ_{pol} is the angle between the incident electric field vector and the x axis. L is the thickness of a unit cell, $L = L_{A1} + L_{A2} + L_B$.

CE-ADI-FDTD method and the conventional method in [64] at CFLN=200 and for various incident wave polarizations. The figure shows that both methods achieve similar levels of accuracy. However, the required CPU time of the proposed CE-ADI-FDTD method at CFLN=200 is 58.2% of the required CPU time of [64]. The proposed method requires much lower CPU time and therefore is more efficient than the conventional method in [64].

Fig. 4.12 further shows that the field intensity is significantly enhanced inside the SBE PhC for all polarizations, due to the slow wave phenomena. However, the amount of field enhancement depends on the incident wave polarization. Specifically, the polarizations $\phi_{pol} = 0^\circ$ and $\phi_{pol} = 90^\circ$ produce the most and least field enhancements, respectively. The field intensities at $\phi_{pol} = 90^\circ$, 156.3° and 261.8° can be increased to match the field intensity at $\phi_{pol} = 0^\circ$ by tuning the orientation angles ϕ_{A1} and ϕ_{A2} of the

Figure 4.12: Time-averaged field intensity $|E|^2$ of a SBE PhC with $N = 11$ for different incident wave polarizations ϕ_{pol} . Continuous line plots with and without marker $\bigcirc$ represent $|E|^2$ values obtained using proposed efficient CE-ADI-FDTD method and CE-ADI-FDTD method presented in [64], respectively.

permittivity tensor using the relation

$$\begin{aligned}\phi_{A1,tuned} &= \phi_{pol,1} - \phi_{pol,2} + \phi_{A1} \\ \phi_{A2,tuned} &= \phi + \phi_{A1,tuned}.\end{aligned}\tag{4.167}$$

The misalignment angle $\phi = \phi_{A2} - \phi_{A1}$ is kept constant so as to maintain the polarization-independent unit transmittance at the Fabry-Perot resonance and the SBE of dispersion relation in Fig. 4.11. In (4.167), the field intensity obtained with $\phi_{pol,1}$ is to be matched to that obtained with $\phi_{pol,2}$. To illustrate this matching, Fig. 4.13(a) plots the field intensities obtained with $\phi_{pol,1} = 90^\circ, 156.3^\circ$ and 261.8° that are enhanced to match that of $\phi_{pol,2} = 0^\circ$. The corresponding tuned angles ϕ_{A1} and ϕ_{A2} are indicated in the figure. In contrast, Fig. 4.13(b) plots the field intensities obtained with $\phi_{pol,1} = 0^\circ, 156.3^\circ$ and 261.8° that are reduced to match that of $\phi_{pol,2} = 90^\circ$.

Figure 4.13: Field intensity achieved inside the SBE PhC for different polarizations matched to a) $\phi_{pol,2} = 0^\circ$ and b) $\phi_{pol,2} = 90^\circ$.

4.3.3 Experiment 3: 2-D Tunable Magnetic Photonic Crystal Cavity

In this section, we validate the proposed 2-D extension of the CE-ADI-FDTD for efficient modeling of a 2-D tunable magnetic photonic crystal (PhC) cavity [102]. A 5×5 PhC consisting of dielectric rods with lattice constant a and radius $r = 0.3a$ in free space is considered. The dielectric rods have a scalar permittivity of 12.25. The centre defect rod is of ferrite material with an anisotropic permeability tensor. The remaining rods have free space permeability. The fine-grid meshing of the 2-D PhC is highlighted in Fig. 4.14, in which the defect centre rod is shown in red. Due to the centre defect, a defect mode is created within the bandgap (bandgap is between normalized frequency $\frac{\omega a}{2\pi c} = 0.404 - 0.508$ [102]). The resonant frequency of this defect mode can be tuned by means of the external biasing magnetic field [102].

The change of the defect mode frequency versus the external biasing magnetic field ω_0 is analyzed using the proposed CE-ADI-FDTD method. The following simulation parameters are used in the CE-ADI-FDTD method: $a = 583\text{nm}$, uniform cell size of $\Delta = 19.4\text{nm}$ and time step size of $\Delta t = \text{CFLN} \frac{\Delta}{c\sqrt{2}}$ where for conventional FDTD, the

Figure 4.14: Fine-grid meshing of 2-D magnetic PhC.

Figure 4.15: Variation of 2-D PhC defect mode frequency for different values of external biasing magnetic field $\omega_0 = \omega_{0,c} \frac{2\pi c}{a}$.

CFLN is set to 1. For the CE-ADI-FDTD simulation, CFLN is set to 4. 10 layer PML boundaries are used to terminate the simulation domain. A modulated Gaussian source $e^{-(\frac{t-t_0}{T_0})^2} \cos(\omega_c(t-t_0))$ where $t_0 = 120\text{fs}$, $T_0 = 30\text{fs}$ and $\omega_c = 0.46 \frac{2\pi c}{a}$ is used to excite the cavity. The ferrite material is assumed lossless. The saturation magnetization ($\omega_m = \gamma\mu_0 M_s$) is fixed to $\omega_m = 0.5 \frac{2\pi c}{a}$. The biasing magnetic field strength ($\omega_0 = \gamma\mu_0 H_0$) is set to $\omega_0 = \omega_{0,c} \frac{2\pi c}{a}$ and varied for $0.75 \leq \omega_{0,c} \leq 1.5$. At an observation point, 5 cells off the cavity centre, the E_z field is recorded and Fourier transformed to analyze the resonant

frequency. The spectrum of E_z at different biasing magnetic field strength ω_0 is plotted in Fig. 4.15. As can be seen, the resonant frequencies of the defect mode are verified to lie within the bandgap of $0.404 - 0.508$ [102]. In addition, as the biasing field strength is varied, the resonant frequency of the defect mode is verified to change. The proposed CE-ADI-FDTD method can thus be used to model the 2D magnetic PhC while requiring fewer temporal iterations.

4.4 Concluding Remarks

In conclusion, this chapter has presented four extensions of the CE-ADI-FDTD method for the efficient analysis of anisotropic periodic media. The ADI schemes in these four extensions were generally formulated using an efficient ADI splitting formulae, that generally produces update equations with fewer and simpler RHS terms, making it easy and efficient to implement the CE-ADI-FDTD method. The CE-ADI-FDTD method was first extended for modeling inhomogeneous saturated ferrite with anisotropic permittivity tensor and ferrite loss. Auxiliary differential equation was used to model the saturated ferrite. Next, the CE-ADI-FDTD method was extended to model inhomogeneous media with anisotropic permittivity tensor and material gain. To model the field interactions with gain medium, a polarization term was added to the magnetic curl equations. The evolution of the polarization term was described by a 'Harmonic oscillator' equation, in which, the polarization was driven by the electric field itself as well as the microscopic carrier distributions. A four-level atomic system was used to model the distribution of carriers over four discrete energy levels. The changes in carrier distributions over these four levels are governed by rate equations in time-domain. A more efficient formulation of the conventional CE-ADI-FDTD method for nonmagnetic periodic structures (without gain) was then presented. A flops count and number of RHS

terms comparison was made with the conventional CE-ADI-FDTD method, in which, it was noted that the proposed method (obtained via efficient ADI splitting formulae) has flops count and number of RHS terms reduced by about half times of those in the conventional method. A 2-D extension of the CE-ADI-FDTD method was finally presented for modeling 2-D magnetic periodic structures composed of saturated ferrite.

Numerical validation of the extended CE-ADI-FDTD methods have been performed using examples of both 1-D and 2-D PhC structures. The extended CE-ADI-FDTD method for 1-D magnetic PhCs was first validated by an example of a magnetic PhC displaying a stationary inflection point. The proposed CE-ADI-FDTD method for 1-D nonmagnetic PhCs with gain material was then validated by an example of laser dye doped cholesteric liquid crystal, in which, circularly polarized lasing was verified at the edge of the stop band. The more efficiently formulated CE-ADI-FDTD method for nonmagnetic PhCs (without gain) was then validated by an example of a nonmagnetic PhC with split band edges (SBE) in the band diagram. It was further highlighted that the field enhancement effect in SBE PhC can be optimized for an incident wave polarization by properly tuning the orientation angles of the anisotropy axes of the SBE PhC layers. The 2-D extended CE-ADI-FDTD method was finally validated by an example of a 2-D tunable magnetic PhC cavity. Due to the centre defect by ferrite material infiltration, defect mode is verified to form. The defect mode resonant frequency can be tuned by varying the external biasing magnetic field strength.

Chapter 5

Analytic Fields with Higher-Order Compensations for 3-D FDTD TF/SF Formulation

5.1 Introduction

In Section 2.4, several methods were reviewed to compute incident fields for the TF/SF formulation in Yee's FDTD scattering analysis of structures that can be anisotropic. These methods can generally be categorized as 1-D auxiliary grid based methods as well as frequency-domain and time-domain analytic based methods. The former method is generally used to excite a plane wave while the latter analytic methods can be used to excite both plane wave and non-plane waves for example focused beams. Time-domain analytic methods can utilize less memory storage compared to frequency-domain analytic methods. However, they are less accurate due to approximation of numerical artifacts, in the time-domain. Given the usefulness of time-domain analytic methods in

sourcing both plane and non-plane waves while consuming lesser memory, it would be advantageous to improve on its accuracy.

In this chapter, we present an improved time-domain analytic method for computing incident fields in the Yee's TF/SF formulation and demonstrate its ability in sourcing a focused beam. The proposed method improves on the accuracy of [91] in two ways. Firstly, it enhances the FDTD dispersion compensation with a higher-order approximation of the numerical wavenumber and secondly, it accounts for the lack of orthogonality between the frequency-dependent field polarizations and the wavevector, which was not accounted for in [91] and [92]. The higher-order dispersion and polarization compensations are included into a set of analytic field expressions that can then be used to practically compute the required incident fields at every time step, unlike frequency-domain methods which require the incident fields to be synthesized and stored before the start of the FDTD simulation.

This chapter begins in Section 5.2 with a Fourier analysis of FDTD update equations. In this analysis, three characteristics of plane wave propagation in the FDTD grid are discussed: numerical (FDTD) dispersion, impedance and polarization. Of them, numerical dispersion and polarization should be accounted for in the analytic expressions of an incident wave. Next, Sections 5.3.1 and 5.3.2 present the higher-order numerical wavenumber and frequency-dependent field polarization compensations, respectively. The time-domain analytic fields of a plane wave and focused beam with higher-order compensations are then presented in Sections 5.3.3 and 5.3.4, respectively. Formulations that facilitate their implementation are provided in Section 5.4. Section 5.5 next presents an error analysis of phase approximations. Numerical experiments of both 3-D plane wave and focused beam are presented in Section 5.6 to demonstrate the performance of the proposed method. Section 5.7 finally provides the conclusion.

5.2 FDTD Fourier Analysis

In this section, we present the Fourier analysis of FDTD update equations. Specifically, we analyze the numerical dispersion, wave impedance and polarization relations of a plane wave propagation in free space FDTD grid. This analysis will be used in subsequent sections to derive and verify the proposed analytic expressions.

Let the electric and magnetic fields at a position $\mathbf{r}_{i,j,k} = i\Delta x\hat{x} + j\Delta y\hat{y} + k\Delta z\hat{z}$ from a reference point be represented in Fourier domain as

$$\hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, \omega) = \hat{\mathbf{E}}^{ref}(\omega) e^{-j\tilde{\mathbf{k}} \cdot \mathbf{r}_{i,j,k}} \quad (5.1)$$

$$\hat{\mathbf{H}}(\mathbf{r}_{i,j,k}, \omega) = \hat{\mathbf{H}}^{ref}(\omega) e^{-j\tilde{\mathbf{k}} \cdot \mathbf{r}_{i,j,k}} \quad (5.2)$$

for a plane wave propagating in a free space FDTD grid. The numerical wavevector $\tilde{\mathbf{k}}$ is given as $\tilde{\mathbf{k}} = \tilde{k}\mathbf{U}_k$ where $\mathbf{U}_k = \cos\phi \sin\theta\hat{x} + \sin\phi \sin\theta\hat{y} + \cos\theta\hat{z}$ is the propagation direction and $\tilde{k}$ is the numerical wavenumber. The vector components of $\tilde{\mathbf{k}}$ are $\tilde{k}_\xi$ for $\xi = x, y, z$. The angle θ is relative to the z axis and the angle ϕ is relative to the x axis when projected in the xy plane. The electric and magnetic fields at the reference point, $\hat{\mathbf{E}}^{ref}(\omega)$ and $\hat{\mathbf{H}}^{ref}(\omega)$, are related through the following vector equations that can be deduced by Fourier analysis of FDTD update equations [86]:

$$j\Omega\epsilon\hat{\mathbf{E}}^{ref}(\omega) = j\hat{\mathbf{H}}^{ref}(\omega) \times \mathbf{K} \quad (5.3)$$

$$j\Omega\mu\hat{\mathbf{H}}^{ref}(\omega) = j\mathbf{K} \times \hat{\mathbf{E}}^{ref}(\omega) \quad (5.4)$$

where

$$\begin{aligned}\Omega &= \frac{2}{\Delta t} \sin\left(\frac{\omega \Delta t}{2}\right) \\ \mathbf{K} &= K_x \hat{x} + K_y \hat{y} + K_z \hat{z} \\ &= \frac{2}{\Delta x} \sin\left(\frac{\tilde{k}_x \Delta x}{2}\right) \hat{x} + \frac{2}{\Delta y} \sin\left(\frac{\tilde{k}_y \Delta y}{2}\right) \hat{y} + \frac{2}{\Delta z} \sin\left(\frac{\tilde{k}_z \Delta z}{2}\right) \hat{z}.\end{aligned}\tag{5.5}$$

5.2.1 Numerical Dispersion

By solving for $\hat{\mathbf{E}}^{ref}$ in (5.3) and using it to eliminate $\hat{\mathbf{E}}^{ref}$ from (5.4), one obtains

$$j\Omega\mu\hat{\mathbf{H}}^{ref}(\omega) = \frac{j}{\Omega\epsilon}(\mathbf{K} \times (\hat{\mathbf{H}}^{ref}(\omega) \times \mathbf{K})).\tag{5.6}$$

Expanding the cross products yields,

$$j\Omega\mu\hat{\mathbf{H}}^{ref}(\omega) = \frac{j}{\Omega\epsilon}(\hat{\mathbf{H}}^{ref}(\omega)(\mathbf{K} \cdot \mathbf{K}) - \mathbf{K}(\mathbf{K} \cdot \hat{\mathbf{H}}^{ref}(\omega))).\tag{5.7}$$

Given that $\mathbf{K} \cdot \mathbf{K} = |\mathbf{K}|^2$ and $\mathbf{K} \cdot \hat{\mathbf{H}}^{ref}(\omega) = 0$, (5.7) can be expressed as

$$j\Omega\mu\hat{\mathbf{H}}^{ref}(\omega) = \frac{j}{\Omega\epsilon}\hat{\mathbf{H}}^{ref}(\omega)|\mathbf{K}|^2.\tag{5.8}$$

Since (5.8) is true for every component of $\hat{\mathbf{H}}^{ref}(\omega)$, it can be eliminated to give the dispersion relation in compact form as

$$\Omega^2\mu\epsilon = |\mathbf{K}|^2\tag{5.9}$$

or in expanded form as

$$\frac{S_x^2 \sin^2(\frac{\tilde{k}_x \Delta x}{2})}{\sin^2(\frac{\omega \Delta t}{2})} + \frac{S_y^2 \sin^2(\frac{\tilde{k}_y \Delta y}{2})}{\sin^2(\frac{\omega \Delta t}{2})} + \frac{S_z^2 \sin^2(\frac{\tilde{k}_z \Delta z}{2})}{\sin^2(\frac{\omega \Delta t}{2})} = 1, \quad (5.10)$$

where $S_\xi = \frac{c \Delta t}{\Delta \xi}$ for $\xi = x, y, z$.

The numerical dispersion relation (5.10) reduces to its physical form specifically for two cases: 1) in the limit of small discretization ($\Delta x, \Delta y, \Delta z, \Delta t \rightarrow 0$) and 2) propagation direction satisfies the relation $\Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$ with a corresponding time step size set to the Courant-limit time step. The numerical wavenumber reduces to the physical wavenumber as well. These two cases are verified next.

Consider the first case. The series expansion of sin terms in (5.10) yields

$$\begin{aligned} & \frac{c^2 \left[\left(\frac{\tilde{k}_x}{2}\right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_x}{2}\right)^4 \Delta x^2 + O(\tilde{k}_x^6 \Delta x^4) \right]}{\left(\frac{\omega}{2}\right)^2 - \frac{1}{3} \left(\frac{\omega}{2}\right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} + \frac{c^2 \left[\left(\frac{\tilde{k}_y}{2}\right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_y}{2}\right)^4 \Delta y^2 + O(\tilde{k}_y^6 \Delta y^4) \right]}{\left(\frac{\omega}{2}\right)^2 - \frac{1}{3} \left(\frac{\omega}{2}\right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} \\ & + \frac{c^2 \left[\left(\frac{\tilde{k}_z}{2}\right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_z}{2}\right)^4 \Delta z^2 + O(\tilde{k}_z^6 \Delta z^4) \right]}{\left(\frac{\omega}{2}\right)^2 - \frac{1}{3} \left(\frac{\omega}{2}\right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} = 1. \end{aligned} \quad (5.11)$$

In the limit of small discretization ($\Delta x, \Delta y, \Delta z, \Delta t \rightarrow 0$), (5.11) can be expressed as

$$\begin{aligned} \lim_{\Delta x, \Delta y, \Delta z, \Delta t \rightarrow 0} \{ & \frac{c^2 \left[\left(\frac{\tilde{k}_x}{2}\right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_x}{2}\right)^4 \Delta x^2 + O(\tilde{k}_x^6 \Delta x^4) \right]}{\left(\frac{\omega}{2}\right)^2 - \frac{1}{3} \left(\frac{\omega}{2}\right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} \\ & + \frac{c^2 \left[\left(\frac{\tilde{k}_y}{2}\right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_y}{2}\right)^4 \Delta y^2 + O(\tilde{k}_y^6 \Delta y^4) \right]}{\left(\frac{\omega}{2}\right)^2 - \frac{1}{3} \left(\frac{\omega}{2}\right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} \\ & + \frac{c^2 \left[\left(\frac{\tilde{k}_z}{2}\right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_z}{2}\right)^4 \Delta z^2 + O(\tilde{k}_z^6 \Delta z^4) \right]}{\left(\frac{\omega}{2}\right)^2 - \frac{1}{3} \left(\frac{\omega}{2}\right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} \} = 1. \end{aligned} \quad (5.12)$$

Applying the rules for limit evaluation of a sum [131] on (5.12) gives

$$\begin{aligned}
& \lim_{\Delta x, \Delta t \rightarrow 0} \frac{c^2 \left[\left(\frac{\tilde{k}_x}{2} \right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_x}{2} \right)^4 \Delta x^2 + O(\tilde{k}_x^6 \Delta x^4) \right]}{\left(\frac{\omega}{2} \right)^2 - \frac{1}{3} \left(\frac{\omega}{2} \right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} \\
& + \lim_{\Delta y, \Delta t \rightarrow 0} \frac{c^2 \left[\left(\frac{\tilde{k}_y}{2} \right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_y}{2} \right)^4 \Delta y^2 + O(\tilde{k}_y^6 \Delta y^4) \right]}{\left(\frac{\omega}{2} \right)^2 - \frac{1}{3} \left(\frac{\omega}{2} \right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} \\
& + \lim_{\Delta z, \Delta t \rightarrow 0} \frac{c^2 \left[\left(\frac{\tilde{k}_z}{2} \right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_z}{2} \right)^4 \Delta z^2 + O(\tilde{k}_z^6 \Delta z^4) \right]}{\left(\frac{\omega}{2} \right)^2 - \frac{1}{3} \left(\frac{\omega}{2} \right)^4 \Delta t^2 + O(\omega^6 \Delta t^4)} = 1. \tag{5.13}
\end{aligned}$$

Next, applying the rules for limit evaluation of a quotient [131] on (5.13) gives

$$\begin{aligned}
& \frac{\lim_{\Delta x \rightarrow 0} \{ c^2 \left[\left(\frac{\tilde{k}_x}{2} \right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_x}{2} \right)^4 \Delta x^2 + O(\tilde{k}_x^6 \Delta x^4) \right] \}}{\lim_{\Delta t \rightarrow 0} \{ \left(\frac{\omega}{2} \right)^2 - \frac{1}{3} \left(\frac{\omega}{2} \right)^4 \Delta t^2 + O(\omega^6 \Delta t^4) \}} \\
& + \frac{\lim_{\Delta y \rightarrow 0} \{ c^2 \left[\left(\frac{\tilde{k}_y}{2} \right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_y}{2} \right)^4 \Delta y^2 + O(\tilde{k}_y^6 \Delta y^4) \right] \}}{\lim_{\Delta t \rightarrow 0} \{ \left(\frac{\omega}{2} \right)^2 - \frac{1}{3} \left(\frac{\omega}{2} \right)^4 \Delta t^2 + O(\omega^6 \Delta t^4) \}} \\
& + \frac{\lim_{\Delta z \rightarrow 0} \{ c^2 \left[\left(\frac{\tilde{k}_z}{2} \right)^2 - \frac{1}{3} \left(\frac{\tilde{k}_z}{2} \right)^4 \Delta z^2 + O(\tilde{k}_z^6 \Delta z^4) \right] \}}{\lim_{\Delta t \rightarrow 0} \{ \left(\frac{\omega}{2} \right)^2 - \frac{1}{3} \left(\frac{\omega}{2} \right)^4 \Delta t^2 + O(\omega^6 \Delta t^4) \}} = 1. \tag{5.14}
\end{aligned}$$

Finally, evaluating the limit in (5.14) and after some rearrangements yields

$$\tilde{k}_x^2 + \tilde{k}_y^2 + \tilde{k}_z^2 = \frac{\omega^2}{c^2} \tag{5.15}$$

Equation (5.15) resembles the dispersion relation in physical free space. Substitution of the components $\tilde{k}_\xi$ for $\xi = x, y, z$ then yields

$$\tilde{k}^2 ((\cos \phi \sin \theta)^2 + (\sin \phi \sin \theta)^2 + (\cos \theta)^2) = \frac{\omega^2}{c^2} \tag{5.16}$$

Substituting $((\cos\phi \sin\theta)^2 + (\sin\phi \sin\theta)^2 + (\cos\theta)^2) = 1$ and taking the square root gives

$$\tilde{k} = \frac{\omega}{c} = k_0. \quad (5.17)$$

The numerical wavenumber thus reduces to the physical wavenumber.

Next, consider the second case. Let $\Delta m = \Delta x \cos\phi \sin\theta = \Delta y \sin\phi \sin\theta = \Delta z \cos\theta$. By substituting Δm in place of $\Delta\xi$ terms (for $\xi = x, y, z$) in the dispersion relation (5.10) and expanding the components $\tilde{k}_\xi$, one obtains

$$\left(\frac{c\Delta t}{\Delta m}\right)^2 \frac{\sin^2(\frac{\tilde{k}\Delta m}{2})}{\sin^2(\frac{\omega\Delta t}{2})} = 1. \quad (5.18)$$

The Courant-limit time step relation is given by [3]

$$\Delta t = \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}. \quad (5.19)$$

Substituting Δm in place of $\Delta\xi$ terms in (5.19) yields

$$\frac{c\Delta t}{\Delta m} = 1. \quad (5.20)$$

Substituting (5.20) into (5.18) and taking the square root yields

$$\sin\left(\frac{\tilde{k}\Delta m}{2}\right) = \sin\left(\frac{\omega\Delta t}{2}\right). \quad (5.21)$$

Upon equating the argument in (5.21) and eliminating Δt and Δm with (5.20), it can be deduced that

$$\tilde{k} = \frac{\omega}{c} = k_0. \quad (5.22)$$

The numerical wavenumber thus reduces to the physical wavenumber. Note that the angles in $\Delta m = \Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$ represent propagation at the complementary diagonal angles and for a unity grid aspect ratio, the complementary diagonals are the physical grid diagonals [79].

5.2.2 Impedance

Taking the vector magnitude of both sides of (5.3) and (5.4) gives

$$|\Omega \epsilon \hat{\mathbf{E}}^{ref}(\omega)| = |\hat{\mathbf{H}}^{ref}(\omega) \times \mathbf{K}| \quad (5.23)$$

$$|\Omega \mu \hat{\mathbf{H}}^{ref}(\omega)| = |\mathbf{K} \times \hat{\mathbf{E}}^{ref}(\omega)|. \quad (5.24)$$

Since $\hat{\mathbf{E}}^{ref}$, $\hat{\mathbf{H}}^{ref}$ and $\mathbf{K}$ are mutually orthogonal vectors (as noted from (5.3) and (5.4)), (5.23) and (5.24) can be reexpressed as,

$$\Omega \epsilon |\hat{\mathbf{E}}^{ref}(\omega)| = |\hat{\mathbf{H}}^{ref}(\omega)| |\mathbf{K}| \quad (5.25)$$

$$\Omega \mu |\hat{\mathbf{H}}^{ref}(\omega)| = |\mathbf{K}| |\hat{\mathbf{E}}^{ref}(\omega)|. \quad (5.26)$$

Dividing (5.25) by (5.26) and rearranging yields

$$\frac{|\hat{\mathbf{E}}^{ref}(\omega)|}{|\hat{\mathbf{H}}^{ref}(\omega)|} = \sqrt{\frac{\mu}{\epsilon}}. \quad (5.27)$$

Equation (5.27) is the wave impedance in a free space FDTD grid. It is exactly equal to that in the physical free space.

5.2.3 Polarization

Let the polarization of $\hat{\mathbf{E}}^{ref}(\omega)$ and $\hat{\mathbf{H}}^{ref}(\omega)$ be represented by the unit vectors $\mathbf{U}_{\hat{E}}$ and $\mathbf{U}_{\hat{H}}$, respectively. Let $\mathbf{U}_K$ be the unit vector of $\mathbf{K}$ ($\frac{\mathbf{K}}{|\mathbf{K}|}$) that can be expressed, using $\mathbf{K}$ from (5.5) and $\Omega\sqrt{\mu\epsilon} = |\mathbf{K}|$, as

$$\mathbf{U}_K = \frac{S_x \sin(\frac{\tilde{k}_x \Delta x}{2})}{\sin(\frac{\omega \Delta t}{2})} \hat{x} + \frac{S_y \sin(\frac{\tilde{k}_y \Delta y}{2})}{\sin(\frac{\omega \Delta t}{2})} \hat{y} + \frac{S_z \sin(\frac{\tilde{k}_z \Delta z}{2})}{\sin(\frac{\omega \Delta t}{2})} \hat{z}. \quad (5.28)$$

Note that the components of vector $\mathbf{U}_K$ ($U_{K\xi}$ for $\xi = x, y, z$) correspond to the projection terms $\tilde{p}_\xi$ in [80], [85]. From (5.10), it can be seen that these components also satisfy the projection equality $1 = U_{Kx}^2 + U_{Ky}^2 + U_{Kz}^2$.

From (5.3) and (5.4), a set of equations relating $\mathbf{U}_{\hat{E}}$, $\mathbf{U}_{\hat{H}}$ and $\mathbf{U}_K$ can be arrived at as

$$\mathbf{U}_{\hat{E}} = \mathbf{U}_{\hat{H}} \times \mathbf{U}_K \quad (5.29)$$

$$\mathbf{U}_{\hat{H}} = \mathbf{U}_K \times \mathbf{U}_{\hat{E}}. \quad (5.30)$$

Note that relations $|\mathbf{K}| = \Omega\sqrt{\mu\epsilon}$ and $\frac{|\hat{\mathbf{E}}^{ref}(\omega)|}{|\hat{\mathbf{H}}^{ref}(\omega)|} = \sqrt{\frac{\mu}{\epsilon}}$ were used to obtain (5.29) and (5.30). Equations (5.29) and (5.30) indicate that $\mathbf{U}_{\hat{E}}$, $\mathbf{U}_{\hat{H}}$ and $\mathbf{U}_K$ form a mutually orthogonal set of vectors.

To satisfy (5.29) and (5.30), $\mathbf{U}_{\hat{E}}$ can be specified as [85]

$$\mathbf{U}_{\hat{E}} = \begin{bmatrix} \cos \psi \sin \tilde{\phi} - \sin \psi \cos \tilde{\theta} \cos \tilde{\phi} \\ -\cos \psi \cos \tilde{\phi} - \sin \psi \cos \tilde{\theta} \sin \tilde{\phi} \\ \sin \psi \sin \tilde{\theta} \end{bmatrix} \quad (5.31)$$

in which the FDTD numerical angles $\tilde{\phi}$ and $\tilde{\theta}$ are the direction angles of vector $\mathbf{U}_K$ that can be determined from the following trigonometric relations with the components of vector $\mathbf{U}_K$:

$$\begin{aligned} \cos \tilde{\theta} &= U_{Kz} & \sin \tilde{\theta} &= \sqrt{1 - U_{Kz}^2} \\ \cos \tilde{\phi} &= \frac{U_{Kx}}{\sqrt{1 - U_{Kz}^2}} & \sin \tilde{\phi} &= \frac{U_{Ky}}{\sqrt{1 - U_{Kz}^2}}. \end{aligned} \quad (5.32)$$

The polarization angle ψ is specified with reference to the direction $\mathbf{U}_k \times \hat{z}$. $\mathbf{U}_{\hat{H}}$ can be obtained by replacing $\cos \psi$ and $\sin \psi$ in (5.31) with $\sin \psi$ and $-\cos \psi$, respectively.

In general, the numerical vector $\mathbf{U}_K$ is not parallel (or equal) to the physical direction vector $\mathbf{U}_k$. As such, unlike physical space, the unit vectors $\mathbf{U}_{\hat{E}}$ and $\mathbf{U}_{\hat{H}}$ are not orthogonal to $\mathbf{U}_k$. Furthermore, as noted in (5.28), the components of vector $\mathbf{U}_K$ are generally frequency-dependent. This implies that the trigonometric functions of $\tilde{\phi}$ and $\tilde{\theta}$ in (5.32) and consequently the unit vectors $\mathbf{U}_{\hat{E}}$ and $\mathbf{U}_{\hat{H}}$ are frequency-dependent.

There are three special cases where the vector $\mathbf{U}_K$ reduces to the physical vector $\mathbf{U}_k$. Consequently, $\tilde{\phi}$ and $\tilde{\theta}$ as well as $\mathbf{U}_{\hat{E}}$ and $\mathbf{U}_{\hat{H}}$ reduce to the physical direction angles and unit vectors, respectively. These cases are: 1) in the limit of small discretization, 2) propagation direction is grid-aligned and 3) propagation direction satisfies the relation $\Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$. These three cases are verified next.

Consider the first case. The components of vector $\mathbf{U}_K$ with series expansion of sin terms are

$$\begin{aligned} U_{K\xi} &= \frac{\frac{c\Delta t}{\Delta\xi} \left[\frac{\tilde{k}_\xi \Delta\xi}{2} - \frac{1}{6} \left(\frac{\tilde{k}_\xi \Delta\xi}{2} \right)^3 + O(\tilde{k}_\xi^5 \Delta\xi^5) \right]}{\frac{\omega\Delta t}{2} - \frac{1}{6} \left(\frac{\omega\Delta t}{2} \right)^3 + O(\omega^5 \Delta t^5)} \\ &= \frac{c \left[\frac{\tilde{k}_\xi}{2} - \frac{1}{6} \left(\frac{\tilde{k}_\xi}{2} \right)^3 \Delta\xi^2 + O(\tilde{k}_\xi^5 \Delta\xi^4) \right]}{\frac{\omega}{2} - \frac{1}{6} \left(\frac{\omega}{2} \right)^3 \Delta t^2 + O(\omega^5 \Delta t^4)}. \end{aligned} \quad (5.33)$$

Setting $\Delta\xi = \Delta t = 0$ and substituting $\tilde{k}_\xi = \tilde{k}U_{k\xi}$ then yields

$$U_{K\xi} = \frac{c}{\omega} \tilde{k} U_{k\xi} \quad (5.34)$$

Since, in the limit of small discretization, the numerical wavenumber reduces to the physical wavenumber or $\tilde{k} = \frac{\omega}{c}$ (see (5.17)), (5.34) reduces to

$$U_{K\xi} = \frac{c}{\omega} \frac{\omega}{c} U_{k\xi} = U_{k\xi}. \quad (5.35)$$

Thus, in the limit of small discretization, $\mathbf{U}_K$ reduces to $\mathbf{U}_k$.

Next, consider the second case. Assuming that the propagation direction is along ξ direction, $\mathbf{U}_K$ is expressed as

$$\mathbf{U}_K = \frac{S_\xi \sin\left(\frac{\tilde{k}\Delta\xi}{2}\right)}{\sin\left(\frac{\omega\Delta t}{2}\right)} \hat{\xi}. \quad (5.36)$$

Note that relation $\tilde{k} = \tilde{k}_\xi$ has been included in (5.36). The dispersion relation for grid aligned propagation can be deduced from (5.10) as

$$\frac{S_\xi^2 \sin^2\left(\frac{\tilde{k}\Delta\xi}{2}\right)}{\sin^2\left(\frac{\omega\Delta t}{2}\right)} = 1. \quad (5.37)$$

Substituting the square root of (5.37) into (5.36) yields

$$\mathbf{U}_K = \hat{\xi}. \quad (5.38)$$

Hence, for grid aligned propagation, $\mathbf{U}_K$ reduces to $\mathbf{U}_k$ that is in the direction of ξ .

Finally, consider the third case. Let the propagation direction be one that satisfies the relation $\Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$. Letting $\Delta m = \Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$ and substituting Δm for $\Delta \xi$ terms in expression of $\mathbf{U}_K$ in (5.28), yields

$$\begin{aligned} \mathbf{U}_K = & \left(\frac{c\Delta t}{\Delta m} \right) \frac{\sin(\frac{\tilde{k}\Delta m}{2})}{\sin(\frac{\omega\Delta t}{2})} \cos \phi \sin \theta \hat{x} + \left(\frac{c\Delta t}{\Delta m} \right) \frac{\sin(\frac{\tilde{k}\Delta m}{2})}{\sin(\frac{\omega\Delta t}{2})} \sin \phi \sin \theta \hat{y} \\ & + \left(\frac{c\Delta t}{\Delta m} \right) \frac{\sin(\frac{\tilde{k}\Delta m}{2})}{\sin(\frac{\omega\Delta t}{2})} \cos \theta \hat{z}. \end{aligned} \quad (5.39)$$

The dispersion relation for such a propagation direction has been derived in (5.18). Substituting its square root into (5.39) gives

$$\mathbf{U}_K = \cos \phi \sin \theta \hat{x} + \sin \phi \sin \theta \hat{y} + \cos \theta \hat{z}, \quad (5.40)$$

where the right-hand side is the vector $\mathbf{U}_k$. Hence, the vector $\mathbf{U}_K$ reduces to $\mathbf{U}_k$ when the propagation direction is one that satisfies the relation $\Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$. Note that the time step size was not assumed to be the Courant-limit time step (this applies to second case as well).

In this section, we have presented the Fourier analysis of FDTD update equations. From the analysis, we have noted that unlike physical space, a plane wave propagates in the FDTD grid with two numerical effects: frequency and propagation direction de-

pendent numerical wavenumber due to grid dispersion and frequency-dependent field polarizations. In addition, we have noted that for special cases, the numerical wavenumber and polarizations reduce to those in physical space. In the following sections, we present approximations of these two numerical effects and their compensations in the time-domain analytic field expressions of a plane wave and focused beam.

5.3 Formulation

5.3.1 Higher-order Numerical Wavenumber Approximation

In this section, we present an improved approximation of $\tilde{k}$ from 3rd order (see (2.48)) to 5th order. By increasing the order of approximation of $\tilde{k}$, the dispersion compensation can be improved.

Let $\tilde{k}$ be related to the physical wavenumber $k_0 = \frac{\omega}{c}$ by a factor δ ($\tilde{k} = \frac{\omega}{c}\delta$), that is assumed real. By substituting the vector components of $\tilde{\mathbf{k}} = \frac{\omega}{c}\delta\mathbf{U}_k$ into (5.10) and then performing the series expansion of the terms $\frac{\sin^2 \frac{\tilde{k}_z \Delta z}{2}}{\sin^2 \frac{\omega \Delta t}{2}}$ in (5.10), one can obtain the following expression:

$$\begin{aligned} & \delta^2 + \left(\frac{\delta^2}{12} - \frac{\delta^4 P_2}{12c^2 \Delta t^2} \right) (\omega \Delta t)^2 \\ & + \left(\frac{\delta^2}{240} - \frac{\delta^4 P_2}{144c^2 \Delta t^2} + \frac{\delta^6 P_4}{360c^4 \Delta t^4} \right) (\omega \Delta t)^4 + O((\omega \Delta t)^6) = 1 \end{aligned} \quad (5.41)$$

where

$$P_2 = \Delta x^2 \cos^4 \phi \sin^4 \theta + \Delta y^2 \sin^4 \phi \sin^4 \theta + \Delta z^2 \cos^4 \theta$$

$$P_4 = \Delta x^4 \cos^6 \phi \sin^6 \theta + \Delta y^4 \sin^6 \phi \sin^6 \theta + \Delta z^4 \cos^6 \theta.$$

Before presenting the 5th order approximation of $\tilde{k}$, we illustrate how a 3rd order approximation of $\tilde{k}$, similar to that in (2.48), can be attained from (5.41). First, an approximation of δ correct to $(\omega\Delta t)^2$ is extracted from (5.41) by truncating the $(\omega\Delta t)$ terms that are greater than $(\omega\Delta t)^2$ to yield

$$\delta^4 \frac{P_2(\omega\Delta t)^2}{12c^2\Delta t^2} - \delta^2 \left(1 + \frac{(\omega\Delta t)^2}{12}\right) + 1 \approx 0. \quad (5.42)$$

By solving for δ in (5.42)

$$\delta = \frac{\sqrt{6}c}{\sqrt{P_2}\omega} \sqrt{\left(1 + \frac{(\omega\Delta t)^2}{12}\right) - \sqrt{\left(1 + \frac{(\omega\Delta t)^2}{12}\right)^2 - \frac{P_2\omega^2}{3c^2}}} \quad (5.43)$$

and utilizing the approximation $\sqrt{1-x} \approx 1 - \frac{x}{2} - \frac{x^2}{8}$, δ correct to $(\omega\Delta t)^2$ (δ_{2nd}) is arrived at as

$$\delta_{2nd} = 1 + \frac{1}{24} \left(\frac{P_2}{c^2\Delta t^2} - 1 \right) (\omega\Delta t)^2. \quad (5.44)$$

Then, by substituting δ_{2nd} into $\tilde{k} = \frac{\omega}{c}\delta$, an approximation of $\tilde{k}$ correct to $(\omega\Delta t)^3$ ($\tilde{k}_{3rd}$) can be obtained as

$$\tilde{k}_{3rd} = k_0\delta_{2nd} = k_0 + \Delta k_{3rd} \quad (5.45)$$

where

$$\Delta k_{3rd} = \frac{1}{24c\Delta t} \left(\frac{P_2}{c^2\Delta t^2} - 1 \right) (\omega\Delta t)^3 = \frac{\omega^3}{24} \left(\frac{P_2}{c^3} - \frac{\Delta t^2}{c} \right). \quad (5.46)$$

The expression (5.46) has been obtained in (2.48) using a similar approximation procedure as (5.42)-(5.44). It can be viewed as an approximate deviation of the numerical wavenumber $\tilde{k}$ from the physical wavenumber k_0 . This deviation is both frequency and propagation direction dependent.

Next, we present the improved 5th order approximation of $\tilde{k}$. Let the approximate $\tilde{k}$ correct to $(\omega\Delta t)^5$ be denoted as $\tilde{k}_{5th}$. To determine $\tilde{k}_{5th}$ it is possible to follow a similar approximation procedure to obtain $\tilde{k}_{3rd}$ (see (5.42)-(5.46)), where the left-hand side of expression (5.41) is first truncated by keeping terms up to $(\omega\Delta t)^4$, then the δ correct to $(\omega\Delta t)^4$ (δ_{4th}) is solved from a cubic equation and δ_{4th} is finally multiplied with k_0 to obtain $\tilde{k}_{5th}$. However, attaining δ_{4th} via the cubic equation in a simplified form similar to δ_{2nd} can be a demanding task. In what follows, an alternate approach is presented to extract δ_{4th} in a form similar to δ_{2nd} .

Let the approximated δ correct to $(\omega\Delta t)^4$ be written as

$$\delta_{4th} = 1 + \delta_2(\omega\Delta t)^2 + \delta_4(\omega\Delta t)^4. \quad (5.47)$$

The corresponding $\tilde{k}$ correct to $(\omega\Delta t)^5$ can then be expressed as

$$\tilde{k}_{5th} = k_0\delta_{4th} = k_0 + \Delta k_{5th} \quad (5.48)$$

where Δk_{5th} can be written as

$$\Delta k_{5th} = \frac{\delta_2}{c\Delta t}(\omega\Delta t)^3 + \frac{\delta_4}{c\Delta t}(\omega\Delta t)^5. \quad (5.49)$$

Substituting (5.47) into (5.41) and keeping terms up to $(\omega\Delta t)^4$ leads to

$$\begin{aligned} & 1 + \left(\delta_2 2 + \frac{1}{12} - \frac{P_2}{12c^2\Delta t^2}\right)(\omega\Delta t)^2 \\ & + \left(\delta_4 2 + \delta_2^2 + \frac{\delta_2}{6} - \delta_2 \frac{P_2}{3c^2\Delta t^2} + \frac{1}{240} \right. \\ & \left. - \frac{P_2}{144c^2\Delta t^2} + \frac{P_4}{360c^4\Delta t^4}\right)(\omega\Delta t)^4 + O((\omega\Delta t)^6) = 1. \end{aligned} \quad (5.50)$$

To equate the left and right-hand sides of (5.50) at every real $(\omega\Delta t)$, the polynomial coefficients of $(\omega\Delta t)$ should reduce to zero. By setting the coefficients of $(\omega\Delta t)^2$ and $(\omega\Delta t)^4$ in (5.50) to zero, two equations with the two unknowns δ_2 and δ_4 can be formed and are solved as

$$\begin{aligned}\delta_2 &= \frac{1}{24} \left(\frac{P_2}{c^2 \Delta t^2} - 1 \right) \\ \delta_4 &= \frac{1}{1920} - \frac{1}{192} \frac{P_2}{c^2 \Delta t^2} + \frac{7}{1152} \left(\frac{P_2}{c^2 \Delta t^2} \right)^2 - \frac{1}{720} \frac{P_4}{c^4 \Delta t^4}.\end{aligned}\quad (5.51)$$

Notice that δ_2 is equivalent to the $(\omega\Delta t)^2$ coefficient in (5.44). The approximations Δk_{5th} and $\tilde{k}_{5th}$ are finally deduced by substituting δ_2 and δ_4 into (5.49) and (5.48).

The approximation $\tilde{k}_{5th}$ can be verified to reduce to the physical wavenumber k_0 when the FDTD discretization parameters approach zero ($\Delta x, \Delta y, \Delta z, \Delta t \rightarrow 0$) or when the propagation direction satisfies the relation $\Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$ with a corresponding time step size set to the Courant-limit time step. This behaviour of $\tilde{k}_{5th}$ is therefore consistent with that of its analytic counterpart $\tilde{k}$ (verified in Section 5.2.1).

We next analyze the approximation error from $\tilde{k}_{5th}$ by measuring the difference with its analytic counterpart $\tilde{k}$ over a range of frequencies. The analytic $\tilde{k}$ can be determined from (5.10). In this analysis, $\tilde{k}_{5th}$ and $\tilde{k}$ are computed using the following parameters: Uniform cell size and time step size of $\Delta = 5\text{mm}$ and $\Delta t = \frac{\Delta}{c\sqrt{3}}$, respectively, with c being the speed of wave propagation in free space, frequency range of $\omega = 2\pi \times 10^9 - 12\pi \times 10^9 \text{rad/s}$ that corresponds to cells per wavelength (N_λ) of about $60 - 10$ and propagation direction angles of $\phi = 70^\circ$ and $\theta = 30^\circ$. Fig. 5.1 plots the approximation error from $\tilde{k}_{5th}$ in logarithmic scale. Plotted together, for comparison, is the approximation error from $\tilde{k}_{3rd}$ in (5.45). From the figure, it is observed that the approximation error from $\tilde{k}_{5th}$ is generally lower compared to that from $\tilde{k}_{3rd}$. This verifies

Figure 5.1: Plot of $\log_{10}|Error = \tilde{k} - \tilde{k}_{3rd/5th}|$ versus $\log_{10}(\omega\Delta t)$ for propagation direction of $\phi = 70^\circ$ and $\theta = 30^\circ$.

that $\tilde{k}_{5th}$ is a better approximation than $\tilde{k}_{3rd}$. Furthermore, the slope of the logarithmic error plots corresponding to $\tilde{k}_{3rd}$ and $\tilde{k}_{5th}$ are 5 and 7, respectively. This verifies their respective 3rd and 5th order accuracy.

5.3.2 Frequency-Dependent Field Polarization Compensation

As highlighted in Section 5.2.3, the incident fields in the FDTD grid are polarized in a direction orthogonal to $\mathbf{U}_K$. In general, the frequency-dependent unit vector $\mathbf{U}_K$ is not the same as the physical direction vector $\mathbf{U}_k$. The field polarizations can be specified for example by $\mathbf{U}_{\hat{E}}$ in (5.31), in which the trigonometric functions of $\tilde{\phi}$ and $\tilde{\theta}$ are related to components of vector $\mathbf{U}_K$ and are generally frequency-dependent. In this section, we present polynomial approximations of the trigonometric functions of $\tilde{\phi}$ and $\tilde{\theta}$ that can be subsequently used to estimate the incident field polarizations, for example $\mathbf{U}_{\hat{E}}$. The inverse Fourier transform of the estimated polarization vector then yields a time-domain operator that can compensate for the frequency-dependent field polarizations in the FDTD grid.

Each component of vector $\mathbf{U}_K$ is first estimated as a polynomial correct to ω^4 from the series expansion of $\frac{\sin \frac{\tilde{k}_\xi \Delta \xi}{2}}{\sin \frac{\omega \Delta t}{2}}$ with $\tilde{k}_\xi \approx \tilde{k}_{5th} U_{k\xi}$ for $\xi = x, y, z$. The estimated components of vector $\mathbf{U}_K$ are then substituted into (5.32) and using the approximations $\sqrt{1-x} \approx 1 - \frac{x}{2} - \frac{x^2}{8}$ and $\frac{1}{1-x} \approx 1 + x + x^2$, the polynomial approximations of trigonometric functions of $\tilde{\phi}$ and $\tilde{\theta}$, correct to $(\omega \Delta t)^4$, are attained as

$$\begin{aligned}\cos \tilde{\theta}_{4th} &= (\cos \theta)(1 + c_2^t(\omega \Delta t)^2 + c_4^t(\omega \Delta t)^4) \\ \sin \tilde{\theta}_{4th} &= (\sin \theta)(1 + s_2^t(\omega \Delta t)^2 + s_4^t(\omega \Delta t)^4) \\ \cos \tilde{\phi}_{4th} &= (\cos \phi)(1 + c_2^p(\omega \Delta t)^2 + c_4^p(\omega \Delta t)^4) \\ \sin \tilde{\phi}_{4th} &= (\sin \phi)(1 + s_2^p(\omega \Delta t)^2 + s_4^p(\omega \Delta t)^4),\end{aligned}\tag{5.52}$$

with the closed-form coefficients $c_{2,4}^{t,p}$ and $s_{2,4}^{t,p}$ listed in Appendix B.

The approximated numerical angles $\tilde{\phi}_{4th}$ and $\tilde{\theta}_{4th}$ in (5.52) can be verified to reduce to the physical angles ϕ and θ when $\Delta x, \Delta y, \Delta z, \Delta t \rightarrow 0$, or when the propagation direction is either grid-aligned or satisfies the relation $\Delta x \cos \phi \sin \theta = \Delta y \sin \phi \sin \theta = \Delta z \cos \theta$. This behaviour of $\tilde{\phi}_{4th}$ and $\tilde{\theta}_{4th}$ is consistent with that of its analytic counterparts $\tilde{\phi}$ and $\tilde{\theta}$ (verified in Section 5.2.3).

Next, we analyze the approximation errors from the approximated trigonometric functions of $\tilde{\phi}$ and $\tilde{\theta}$ by computing their differences with their respective analytic counterparts in (5.32) across a range of frequencies. For example, the error from the frequency-independent approximation of $\cos \tilde{\theta}$ is denoted as $Error_{\cos \tilde{\theta}} = \cos \tilde{\theta} - \cos \theta$. In this analysis, the following parameters are specified: Uniform cell size of $\Delta = 5\text{mm}$ and time step size of $\Delta t = \frac{\Delta}{c\sqrt{3}}$, frequency range of $\omega = 2\pi \times 10^9 - 12\pi \times 10^9 \text{rad/s}$ and propagation direction angles of $\phi = 70^\circ$ and $\theta = 30^\circ$. Fig. 5.2 plots, in logarithmic scale, the absolute errors produced from each approximated function in (5.52) and the

Figure 5.2: Plot of $\log_{10}|Error|$ versus $\log_{10}(\omega\Delta t)$. Dash- and dot-lines represent errors from trigonometric function approximations correct to $(\omega\Delta t)^0$ and $(\omega\Delta t)^4$, respectively. 'o', '▷', '◁' and '+' represent errors from $\sin\tilde{\theta}$, $\cos\tilde{\theta}$, $\cos\tilde{\phi}$ and $\sin\tilde{\phi}$ approximations, respectively. Slope of dash- and dot-lines are 2 and 6, respectively.

errors produced from the frequency-independent approximations of (5.32). From the figure, we observe that the approximation errors from (5.52) are generally lower compared to that produced from the frequency-independent approximations. Specifically, at $\omega = 12\pi \times 10^9 \text{ rad/s}$ ($N_\lambda = 10$), the maximum error produced from the frequency-independent approximations is approximately 10^3 times more than that produced from (5.52). From the figure, we further observe that the slope of the logarithmic error plots from the frequency-independent approximations and the approximations in (5.52) are 2 and 6, respectively. This verifies the $(\omega\Delta t)^4$ accuracy of the approximated functions in (5.52).

By substituting the FDTD trigonometric functions in (5.31) with their respective approximated functions in (5.52), the electric field polarization vector in the FDTD grid, for example $\mathbf{U}_{\hat{E}}$, can now be estimated correct to $(\omega\Delta t)^4$ as

$$\mathbf{U}_{\hat{E},4th} = \mathbf{U}_E + \Delta\mathbf{U}_{E,2}(\omega\Delta t)^2 + \Delta\mathbf{U}_{E,4}(\omega\Delta t)^4. \quad (5.53)$$

Figure 5.3: Plot of $\log_{10}(\text{Dot Product Error})$ versus $\log_{10}(\omega \Delta t)$.

The vector coefficients $\Delta \mathbf{U}_{E,2}$ and $\Delta \mathbf{U}_{E,4}$ for a plane wave are listed in Appendix C. $\mathbf{U}_E$ is the frequency-independent polarization vector in physical space, obtained simply by replacing $\tilde{\phi}$ and $\tilde{\theta}$ in (5.31) with ϕ and θ , respectively. To analyze the approximation errors, Fig. 5.3 plots the logarithmic dot product errors $\log_{10}|\mathbf{U}_E \cdot \mathbf{U}_K|$ and $\log_{10}|\mathbf{U}_{\hat{E},4th} \cdot \mathbf{U}_K|$, across a range of frequencies. Note that as the approximated vectors approach $\mathbf{U}_{\hat{E}}$, the dot product errors should approach zero, since $\mathbf{U}_{\hat{E}}$ is orthogonal to $\mathbf{U}_K$. From the figure, we first observe that approximation $\mathbf{U}_{\hat{E},4th}$ produces lower errors compared to that using the physical vector $\mathbf{U}_E$. Secondly, we observe that the slope of the errors produced by $\mathbf{U}_E$ and $\mathbf{U}_{\hat{E},4th}$ are 2 and 6, respectively. This further verifies the $(\omega \Delta t)^4$ accuracy of $\mathbf{U}_{\hat{E},4th}$.

Upon substitutions of $\mathbf{U}_{\hat{E}}$ with $\mathbf{U}_{\hat{E},4th}$ and the magnitude $|\hat{\mathbf{E}}^{ref}(\omega)|$ with the function $G(\omega)$, the electric field at the reference point, $\hat{\mathbf{E}}^{ref}(\omega) = |\hat{\mathbf{E}}^{ref}(\omega)|\mathbf{U}_{\hat{E}}$, can now be estimated as

$$\begin{aligned} \hat{\mathbf{E}}^{ref}(\omega) &\approx G(\omega)\mathbf{U}_{\hat{E},4th} = G(\omega)\mathbf{U}_E \\ &\quad - (j\omega)^2 G(\omega)\Delta \mathbf{U}_{E,2}\Delta t^2 + (j\omega)^4 G(\omega)\Delta \mathbf{U}_{E,4}\Delta t^4. \end{aligned} \quad (5.54)$$

Using the Fourier transform identity $(j\omega)^m \leftrightarrow \frac{\partial^m}{\partial t^m}$, (5.54) can be converted to time-domain as

$$\hat{\mathbf{E}}^{ref}(t) \approx (\mathbf{U}_E - \Delta\mathbf{U}_{E,2}\Delta t^2 \frac{\partial^2}{\partial t^2} + \Delta\mathbf{U}_{E,4}\Delta t^4 \frac{\partial^4}{\partial t^4})g(t) \quad (5.55)$$

where $g(t)$ is the inverse Fourier transform of $G(\omega)$. The $\frac{\partial^m}{\partial t^m}$ operators in (5.55) can be used to compensate in time-domain the frequency dependence of $\mathbf{U}_{\hat{E}}$ and consequently minimize the errors at the TF/SF boundary. A similar approximation can be established for $\hat{\mathbf{H}}^{ref}(t)$ as

$$\hat{\mathbf{H}}^{ref}(t) \approx (\mathbf{U}_H - \Delta\mathbf{U}_{H,2}\Delta t^2 \frac{\partial^2}{\partial t^2} + \Delta\mathbf{U}_{H,4}\Delta t^4 \frac{\partial^4}{\partial t^4})\frac{g(t)}{\eta}, \quad (5.56)$$

where $\mathbf{U}_H$, $\Delta\mathbf{U}_{H,2}$ and $\Delta\mathbf{U}_{H,4}$ can be attained by replacing $\cos\psi$ and $\sin\psi$ in $\mathbf{U}_E$, $\Delta\mathbf{U}_{E,2}$ and $\Delta\mathbf{U}_{E,4}$ with $\sin\psi$ and $-\cos\psi$, respectively. η is the impedance of the wave in the medium.

5.3.3 Analytic Fields of A Plane Wave with Higher-Order Dispersion and Polarization Compensations

Following the derivations in Sections 5.3.1 and 5.3.2, we next present the time-domain analytic field expressions of a plane wave with both higher-order FDTD dispersion and frequency-dependent field polarization compensations. The proposed analytic expressions can be used to calculate the incident fields of a plane wave at the TF/SF boundary with minimal field leakage errors.

The electric field of a plane wave propagating in the FDTD grid is expressed as

$$\begin{aligned}
 \hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, \omega) &= \hat{\mathbf{E}}^{ref}(\omega) e^{-j\tilde{\mathbf{k}} \cdot \mathbf{r}_{i,j,k}} \\
 &= \hat{\mathbf{E}}^{ref}(\omega) e^{-j(k_0 + \Delta k) \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}} \\
 &= \hat{\mathbf{E}}^{ref}(\omega) e^{-jk_0 \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}} e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}},
 \end{aligned} \tag{5.57}$$

where the exponential phase shift term containing the numerical wavenumber has been split into one with the physical wavenumber and one with the numerical deviation. The electric field expression with higher-order dispersion compensation can now be attained by first approximating exponential phase shift term $e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}$ in (5.57) as

$$e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}} \approx 1 - j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k} - \frac{(\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k})^2}{2} + \frac{j(\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k})^3}{3!} \tag{5.58}$$

where the first two real and imaginary terms of the series expansion of $e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}$ are kept. Estimating Δk with the higher-order term Δk_{5th} then gives, in compact form,

$$e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}} \approx 1 + \sum_{r=1}^3 \frac{1}{r!} \gamma_r \sum_{n=0}^r (-1)^n \binom{r}{n} \delta_2^{r-n} \delta_4^n \Delta t^{3r+2n} (j\omega)^{3r+2n} \tag{5.59}$$

where $\gamma_r = (\frac{\mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}{c\Delta t})^r$. Upon substitution of (5.59) into (5.57) and conversion to time-domain using the Fourier identities $(j\omega)^m \leftrightarrow \frac{\partial^m}{\partial t^m}$ and $X(\omega)e^{-j\omega t_0} \leftrightarrow x(t - t_0)$, the following expression for electric field is arrived at

$$\hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, t) \approx C_F \hat{\mathbf{E}}^{ref}(t_D). \tag{5.60}$$

C_F is defined as a higher-order dispersion compensation factor that can be expressed in compact form as

$$C_F = 1 + \sum_{r=1}^3 \frac{1}{r!} \gamma_r \sum_{n=0}^r (-1)^n \binom{r}{n} \delta_2^{r-n} \delta_4^n \Delta t^{3r+2n} \frac{\partial^{3r+2n}}{\partial t^{3r+2n}} \quad (5.61)$$

with $t_D = t - \frac{\mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}{c}$. Note that (5.61) reduces to the lower-order dispersion compensation factor

$$C_F = 1 + \left(\frac{\mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}{c \Delta t} \right) \frac{1}{24} \left(\frac{P_2}{c^2 \Delta t^2} - 1 \right) \Delta t^3 \frac{\partial^3}{\partial t^3}$$

deduced in [91] when $\gamma_2 = \gamma_3 = \delta_4 = 0$. To include the frequency-dependent polarization in (5.60), the reference electric field $\hat{\mathbf{E}}^{ref}(t_D)$ can be substituted from (5.55) into (5.60) to finally yield the electric field with both compensations as

$$\hat{\mathbf{E}}(\mathbf{r}_{i,j,k}, t) \approx (C_F \mathbf{U}_E - C_F \Delta \mathbf{U}_{E,2} \Delta t^2 \frac{\partial^2}{\partial t^2} + C_F \Delta \mathbf{U}_{E,4} \Delta t^4 \frac{\partial^4}{\partial t^4}) g(t_D). \quad (5.62)$$

The magnetic field expression with higher-order dispersion and polarization compensations can be similarly attained as

$$\hat{\mathbf{H}}(\mathbf{r}_{i,j,k}, t) \approx (C_F \mathbf{U}_H - C_F \Delta \mathbf{U}_{H,2} \Delta t^2 \frac{\partial^2}{\partial t^2} + C_F \Delta \mathbf{U}_{H,4} \Delta t^4 \frac{\partial^4}{\partial t^4}) \frac{g(t_D)}{\eta}. \quad (5.63)$$

Equations (5.62)-(5.63) are the proposed analytic expressions that accurately represent a plane wave propagation in the FDTD grid, in time-domain. They include numerical effects, namely, FDTD dispersion and frequency-dependent polarization. The $\frac{\partial^m}{\partial t^m}$ operators along with coefficients δ in C_F and $\Delta \mathbf{U}_E$ are used to compensate in time-domain the frequency dependence of FDTD dispersion and polarization, respectively. They can be used to generate the required fields of an incident plane wave at the TF/SF

boundary with minimal errors.

5.3.4 Analytic Fields of A Focused Beam with Higher-Order Dispersion and Polarization Compensations

In this section, we present the time-domain analytic field expressions of a focused beam with both higher-order FDTD dispersion and frequency-dependent field polarization compensations. The proposed analytic expressions can be used to calculate the incident fields of a focused beam at the TF/SF boundary with minimal field leakage errors.

There are several instances where instead of a plane wave, an incident beam (e.g. Gaussian-like focused beam) may be a more preferred choice of excitation. For example, a focused beam can be used to provide a localized illumination to study the scattering effects within a confined area such as in the case of individual scatterers on a larger target [122]-[124]. Focused beams can also be used to minimize illuminating the edges of a finite-sized scatterer that otherwise, can result in interferences between the diffracted waves, that radiate from the edges of the finite-sized scatterer, and the desired reflected and transmitted waves [90], [125], [126]. Hence, more accurate scattering results such as S parameters can be achieved. An incident beam may also be of interest in modeling part of an optical illumination system such as, the focal area of a converging lens [92].

In general, such beams can be expressed analytically as a finite summation of plane waves, with each plane wave constituent having its own magnitude, phase, polarization and propagation direction. In this work, we consider a focused beam that is formed by an aplanatic lens and propagates in the $-z$ direction towards the focus $\mathbf{F}$ (at the origin)

Figure 5.4: (a) Schematic of a focused beam formed by an aplanatic lens with spherical converging wavefront w and focus F at origin and (b) TF/SF formulation that models the focal area of the converging lens.

with a spherical converging wavefront w [128], [129], as illustrated in Fig. 5.4(a). Such a beam can correspond to that of an optical illumination system, for example a bright-field microscope [92].

Instead of modeling the entire optical system, the TF/SF formulation models the focal area of the converging lens where most of interactions take place between the beam and the object under observation, as highlighted in Fig. 5.4(b). The required incident beam fields at the TF/SF boundary can be analytically determined from its 2-D integral representation. Upon inclusion of numerical artifacts into the original fields [129], the

following integral representation of the incident beam electric field at a point (r_p, θ_p, ϕ_p) around the focus $\mathbf{F}$ can be attained:

$$\hat{\mathbf{E}}(r_p, \theta_p, \phi_p, \omega) = \frac{-jk_0 f}{2\pi} \int_0^{\theta_{max}} \int_0^{2\pi} E_0(\omega) \mathbf{U}_{\hat{E}} e^{-jk_0 r_p \cos \epsilon} e^{-j\Delta k r_p \cos \epsilon} \cos^{\frac{1}{2}} \theta \sin \theta d\phi d\theta. \quad (5.64)$$

where

$$\begin{aligned} \cos \epsilon &= \sin \theta \sin \theta_p \cos(\phi - \phi_p) + \cos \theta \cos \theta_p, \\ \mathbf{U}_{\hat{E}} &= \begin{bmatrix} \cos^2 \tilde{\phi} \cos \tilde{\theta} + \sin^2 \tilde{\phi} \\ \sin \tilde{\phi} \cos \tilde{\phi} (\cos \tilde{\theta} - 1) \\ -\sin \tilde{\theta} \cos \tilde{\phi} \end{bmatrix}. \end{aligned} \quad (5.65)$$

f is the focal length, θ_{max} is the half angular range and the magnitude $E_0(\omega)$ is referenced to the origin.

Expression (5.64) can be interpreted as a summation of plane waves incident from a range of directions (θ, ϕ) [92]. Along each direction, numerical artifacts, namely, FDTD dispersion and frequency-dependent field polarizations, are incorporated in the form of the exponential phase term $e^{-j\Delta k r_p \cos \epsilon}$ and the vector $\mathbf{U}_{\hat{E}}$ that depends on numerical angles $\tilde{\theta}$ and $\tilde{\phi}$ instead of physical angles θ and ϕ , respectively.

Similar to deriving the analytic fields of a plane wave in Section (5.3.3), the $e^{-j\Delta k r_p \cos \epsilon}$ is first approximated in compact form as

$$e^{-j\Delta k r_p \cos \epsilon} \approx 1 + \sum_{r=1}^3 \frac{1}{r!} \gamma_r \sum_{n=0}^r (-1)^n \binom{r}{n} \delta_2^{r-n} \delta_4^n \Delta t^{3r+2n} (-j\omega)^{3r+2n} \quad (5.66)$$

where $\gamma_r = (-\frac{r_p \cos \varepsilon}{c \Delta t})^r$. Note that Δk in $e^{-j \Delta k r_p \cos \varepsilon}$ is approximated by the proposed Δk_{5th} in (5.49).

Next, by substituting the trigonometric functions of $\tilde{\theta}$ and $\tilde{\phi}$ in (5.65) with their respective approximated functions in (5.52), an estimate of the FDTD polarization vector $\mathbf{U}_{\hat{E}}$ can be attained as

$$\mathbf{U}_{\hat{E},4th} = \mathbf{U}_E - (-j\omega)^2 \Delta \mathbf{U}_{E,2} \Delta t^2 + (-j\omega)^4 \Delta \mathbf{U}_{E,4} \Delta t^4, \quad (5.67)$$

correct to $(\omega \Delta t)^4$. The vector coefficients $\Delta \mathbf{U}_{E,2}$ and $\Delta \mathbf{U}_{E,4}$ for a focused beam are listed in Appendix D. $\mathbf{U}_E$ is the frequency-independent polarization vector in physical space, obtained simply by replacing $\tilde{\phi}$ and $\tilde{\theta}$ in (5.65) with ϕ and θ , respectively.

Following the approximations of $e^{-j \Delta k r_p \cos \varepsilon}$ and $\mathbf{U}_{\hat{E}}$ with (5.66) and (5.67), respectively, we next substitute them into the electric field solution (5.64) and use the Fourier identities $(-j\omega)^m \leftrightarrow \frac{\partial^m}{\partial t^m}$ and $X(\omega)e^{-j\omega t_0} \leftrightarrow x(t+t_0)$ to transform it to the following time-domain expression:

$$\begin{aligned} \hat{\mathbf{E}}(r_p, \theta_p, \phi_p, t) = & \frac{f}{2\pi c} \int_0^{\theta_{max}} \int_0^{2\pi} (C_F \mathbf{U}_E - C_F \Delta \mathbf{U}_{E,2} \Delta t^2 \frac{\partial^2}{\partial t^2} \\ & + C_F \Delta \mathbf{U}_{E,4} \Delta t^4 \frac{\partial^4}{\partial t^4}) \dot{E}_0(t_D) \cos^{\frac{1}{2}} \theta \sin \theta d\phi d\theta. \end{aligned} \quad (5.68)$$

where C_F is defined as the dispersion compensation factor

$$C_F = 1 + \sum_{r=1}^3 \frac{1}{r!} \gamma_r \sum_{n=0}^r (-1)^n \binom{r}{n} \delta_2^{r-n} \delta_4^n \Delta t^{3r+2n} \frac{\partial^{3r+2n}}{\partial t^{3r+2n}}$$

and $t_D = t + \frac{r_p \cos \varepsilon}{c}$. Expression (5.68) uses the $\frac{\partial^m}{\partial t^m}$ operators to compensate in time-domain the frequency dependence of the FDTD dispersion and polarization $\mathbf{U}_{\hat{E}}$. The

expression can be used to compute the incident beam electric field at the TF/SF boundary with minimal errors. Note that (5.68) reduces to the electric field expression in physical space [92] when $C_F = 1$ and both $\Delta\mathbf{U}_{E,2}$ and $\Delta\mathbf{U}_{E,4}$ are set to null vectors. A similar expression can be attained for the magnetic field.

5.4 Computing Derivatives of Gaussian Source Functions

In this section, we present formulations that compute the time-derivatives of commonly used Gaussian source functions at a specific time. These formulations can facilitate the implementation of derivatives of source $g(t)$ in the proposed analytic fields (5.62), for a plane wave, and similarly $E_0(t)$ in (5.68), for a focused beam.

For a basic Gaussian source, the value of the n th derivative can be easily computed from the following product between the n th order Hermite polynomial ($H_n(t)$) and the Gaussian [130], [131]:

$$\frac{d^n}{dt^n} e^{-t^2} = (-1)^n e^{-t^2} H_n(t) \quad (5.69)$$

The explicit expression of $H_n(t)$ is not needed for its evaluation since it can be determined via the recurrence relation

$$H_n(t) = 2tH_{n-1}(t) - 2(n-1)H_{n-2}(t) \quad (5.70)$$

and the initial conditions $H_0(t) = 1$ and $H_1(t) = 2t$. For a modulated Gaussian source with variance τ^2 , similar formulations to compute its n th derivative can be obtained, as

follows:

First, using the chain rule, (5.69) can be modified for a Gaussian source with variance τ^2 as

$$\frac{d^n}{dt^n} e^{-\left(\frac{t}{\tau}\right)^2} = \left(\frac{-1}{\tau}\right)^n e^{-\left(\frac{t}{\tau}\right)^2} H_n\left(\frac{t}{\tau}\right). \quad (5.71)$$

Next, let the modulated Gaussian source be $g(t) = u(t)v(t)$ with $u(t) = \sin(\omega_0 t)$ and $v(t) = e^{-\left(\frac{t}{\tau}\right)^2}$. The n th derivative of $u(t)v(t)$ can be written, from Leibnitz' product rule [131], as

$$\frac{d^n}{dt^n} g(t) = \sum_{r=0}^n \binom{n}{r} \frac{d^r}{dt^r} u(t) \frac{d^{n-r}}{dt^{n-r}} v(t). \quad (5.72)$$

By noting that the even and odd r th derivatives of $u(t)$ are $(-1)^{r/2} \omega_0^r \sin(\omega_0 t)$ and $(-1)^{(r-1)/2} \omega_0^r \cos(\omega_0 t)$, respectively, and substituting $\frac{d^{n-r}}{dt^{n-r}} v(t)$ with (5.71), (5.72) can be expressed as

$$\frac{d^n}{dt^n} g(t) = \left(\frac{-1}{\tau}\right)^n e^{-\left(\frac{t}{\tau}\right)^2} (\sin(\omega_0 t) g_n^s(t) + \cos(\omega_0 t) g_n^c(t)) \quad (5.73)$$

where

$$g_n^s(t) = \sum_{\text{even } r} \binom{n}{r} (-1)^{\frac{r}{2}} (\omega_0 \tau)^r H_{n-r}\left(\frac{t}{\tau}\right) \quad (5.74)$$

$$g_n^c(t) = \sum_{\text{odd } r} \binom{n}{r} (-1)^{\frac{r+1}{2}} (\omega_0 \tau)^r H_{n-r}\left(\frac{t}{\tau}\right). \quad (5.75)$$

With the aid of identities $\frac{d}{dt}H_n(\frac{t}{\tau}) = \frac{2n}{\tau}H_{n-1}(\frac{t}{\tau})$ and $(n-r)\binom{n}{r} = n\binom{n-1}{r}$, the terms $g_n^s(t)$ and $g_n^c(t)$ can be deduced, in terms of recurrence relations, as

$$g_n^s(t) = \frac{2t}{\tau}g_{n-1}^s(t) - 2(n-1)g_{n-2}^s(t) + \omega_0\tau g_{n-1}^c(t) \quad (5.76)$$

$$g_n^c(t) = \frac{2t}{\tau}g_{n-1}^c(t) - 2(n-1)g_{n-2}^c(t) - \omega_0\tau g_{n-1}^s(t), \quad (5.77)$$

with the initial conditions $g_0^s(t) = 1$, $g_0^c(t) = 0$, $g_1^s(t) = H_1(\frac{t}{\tau}) = \frac{2t}{\tau}$ and $g_1^c(t) = -\omega_0\tau$. The derivation of (5.76)-(5.77) are presented in Appendix E. Expressions (5.73), (5.76) and (5.77) can be easily programmed to compute the value of the n th derivative of a modulated Gaussian source $g(t) = \sin(\omega_0 t)e^{-(\frac{t}{\tau})^2}$ at a given time. The n th derivative value can then be utilized in (5.62) and (5.68). The above procedures can also be used to obtain similar implementations for other forms of Gaussian source functions such as differentiated and cosine-modulated Gaussian.

The n th derivatives of a modulated Gaussian pulse, computed using the proposed recurrence relations (5.76) and (5.77), are next compared with analytic derivations. This comparison is plotted in Fig. 5.5. The modulated Gaussian pulse is expressed as $\sin(\omega_0(t-t_0))e^{-(\frac{t-t_0}{\tau})^2}$ with $\tau = 75\Delta t$, $t_0 = 600\Delta t$, $\omega_0 = 2\pi \times 10^9 \text{ rad/s}$ and $\Delta t = \frac{1 \times 10^{-2}}{c\sqrt{3}}$. Note that the n th derivatives are normalized by the term Δt^n , respectively. Fig. 5.5 shows good agreement between the proposed method and analytic derivations. Fig. 5.6 further plots the higher-order n th derivatives of the modulated Gaussian pulse, computed using the proposed recurrence relations. The figure shows that the n th derivatives are still bounded in time, even for very large n values of 100. This demonstrates the stability of the proposed recurrence relations.

Figure 5.5: Comparison between n th derivatives of modulated Gaussian pulse computed via proposed recurrence relations and analytic derivations (denoted with marker +).

Figure 5.6: Plot of higher-order n th derivatives of modulated Gaussian pulse, computed using the proposed recurrence relations.

5.5 Phase Error Analysis

In this section, we analyze the phase errors that arise from four types of series approximation of $e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}$, including the proposed approximation used in (5.59). The

approximated phase can be determined from the polar form of the series approximation of $e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}$. The reference phase is defined as $\Theta_{ref} = \Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}$. To facilitate this analysis, let the approximated phase be denoted in general as $\Theta_{l,m}$ where the indices l and m represent the order of approximations of Δk and the series expansion of $e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}$, respectively. The phase error is then denoted as $Error_{l,m} = \Theta_{ref} - \Theta_{l,m}$. We consider the direction of propagation $\theta = 90^\circ$ and $\phi = 0^\circ$ ($\mathbf{U}_k = \hat{x}$) to account for largest dispersion errors [91], [132] and let $x = \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}$. The corresponding phase errors from four types of series approximation of $e^{-j\Delta k \mathbf{U}_k \cdot \mathbf{r}_{i,j,k}}$ can then be expressed as follows:

$$\begin{aligned} Error_{3,1} &= A1(k_0x) + \frac{1}{3}B1^3(k_0x)^3 + O((k_0x)^5) \\ Error_{3,3} &= A1(k_0x) - \frac{1}{30}B1^5(k_0x)^5 + O((k_0x)^7) \\ Error_{5,1} &= A2(k_0x) + \frac{1}{3}B2^3(k_0x)^3 + O((k_0x)^5) \\ Error_{5,3} &= A2(k_0x) - \frac{1}{30}B2^5(k_0x)^5 + O((k_0x)^7), \end{aligned} \quad (5.78)$$

where coefficients $A1$, $A2$, $B1$ and $B2$ depend on the Courant number ($S = \frac{c\Delta t}{\Delta x}$) and cells per wavelength (N_λ) and can be determined from

$$\begin{aligned} Aref &= \frac{N_\lambda}{\pi} \sin^{-1}\left(\frac{1}{S} \sin\left(\frac{S\pi}{N_\lambda}\right)\right) - 1 \\ B1 &= \frac{\pi^2}{6N_\lambda^2}(1 - S^2) \\ B2 &= \frac{\pi^4}{120N_\lambda^4}S^4 - \left(\frac{\pi^2}{6N_\lambda^2} + \frac{\pi^4}{12N_\lambda^4}\right)S^2 + \left(\frac{\pi^2}{6N_\lambda^2} + \frac{3\pi^4}{40N_\lambda^4}\right) \\ A1 &= Aref - B1 \\ A2 &= Aref - B2. \end{aligned}$$

In Fig. 5.7(a), the absolute values of these phase errors are plotted with respect to k_0x . The maximum frequency is assumed as $\omega_{max} \approx \frac{2\pi c}{N_\lambda \Delta x}$ where $N_\lambda = 20$. Uniform cell and

Figure 5.7: Plot of (a) phase errors $|\Theta_{ref} - \Theta_{l,m}|$ for fixed $N_\lambda = 20$ and (b) phase error $|\Theta_{ref} - \Theta_{5,3}|$ for different N_λ values.

time step sizes of $\Delta x = 5\text{mm}$ and $\Delta t = \frac{\Delta x}{c\sqrt{3}}$ are set, respectively.

From the figure, we observe that the phase error produced by $\Theta_{5,3}$, from the approximation proposed in (5.59), is generally the lowest compared to that produced by the other approximated phases and this comparison becomes significant as $k_0 x$ increases. Fig. 5.7(b) further plots the phase error produced by $\Theta_{5,3}$ for different N_λ values. From the figure, we observe that the phase error generally increases as N_λ decreases.

5.6 Numerical Results

In this section, numerical results are presented to validate the proposed analytic field expressions (5.62) and (5.68) that calculate the incident fields at the TF/SF boundary for a plane wave and a focused beam excitation, respectively. The time-derivatives of source functions $g(t)$ and $E_0(t)$ in (5.62) and (5.68), respectively, are computed using (5.73), (5.76) and (5.77).

Figure 5.8: Field leakage in the scattered-field region using modulated Gaussian source with $\omega_0 = 5\pi \times 10^9 \text{ rad/s}$ ($N_\lambda = 10$). The field leakage is below -86 dB using the proposed analytic expressions. Lower-order compensation corresponds to dispersion compensation procedure in [91].

5.6.1 Experiment 1: Plane Wave Excitation

In the first experiment, we initiate a 3-D plane wave into a free space TF region without any scattering objects. The plane wave propagates in the direction $\phi = 70^\circ$ and $\theta = 30^\circ$ with the polarization angle $\psi = 330^\circ$. The entire computational volume is of free space and is meshed with $120 \times 120 \times 120$ uniform grid cells of size 1cm each. The TF region has dimensions $100 \times 100 \times 100$ uniform grid cells and the Mur absorbing boundary condition (ABC) [73] is placed 10 grids away from the TF/SF boundary to terminate the computational volume. The simulation is performed over 1200 time steps of size $\Delta t = \frac{\Delta}{c\sqrt{3}}$ each. The reference point is specified at the centre of the computational volume with the source function $g(t)$ modeled by a modulated Gaussian pulse in time: $\sin(\omega_0(t - t_0))e^{-(\frac{t-t_0}{\tau})^2}$ with $\tau = 75\Delta t$, $t_0 = 600\Delta t$ and two ω_0 values of $2\pi \times 10^9 \text{ rad/s}$ and $5\pi \times 10^9 \text{ rad/s}$. The upper -40 dB magnitude of the source function spectrum corresponds to $N_\lambda = 10$ and 20 when ω_0 is $5\pi \times 10^9 \text{ rad/s}$ and $2\pi \times 10^9 \text{ rad/s}$, respectively.

Figure 5.9: Field leakage in the scattered-field region using modulated Gaussian source with $\omega_0 = 2\pi \times 10^9 \text{ rad/s}$ ($N_\lambda = 20$). The field leakage is below -137.3 dB using the proposed analytic expressions. Lower-order compensation corresponds to dispersion compensation procedure in [91].

To measure the performance of the proposed analytic expressions, the field leakage error at the point (112,112,112) in the SF region is recorded over the entire simulation and is normalized by the peak incident field value. The field leakage error at this point is plotted in Figs. 5.8 and 5.9 for the case of a source function with centre frequencies $\omega_0 = 5\pi \times 10^9 \text{ rad/s}$ and $\omega_0 = 2\pi \times 10^9 \text{ rad/s}$, respectively. Plotted together, for comparison, are the field leakage errors using the expressions presented in [91] that utilizes a lower-order dispersion compensation and does not include compensations for frequency-dependent polarization. From the plots, it can be seen that the proposed analytic expressions can attain field leakage errors below -86 dB and -137.3 dB when the modulated Gaussian source is discretized with N_λ values of 10 and 20, respectively. These error levels are suppressed by amounts of 42.6 dB and 77.6 dB respectively from the corresponding error levels obtained using the expressions in [91]. This verifies the improved performance of the proposed analytic expressions.

Figure 5.10: Grayscale plots of E_x field (in dB) on the $y = 0$ (xz) plane at different time instants (a)-(f). The colorplot bar is restricted to -40 dB.

5.6.2 Experiment 2: Focused Beam Excitation

In the second experiment, we initiate the 3-D focused beam, presented in Section 5.3.4, into a free space TF region without any scattering objects. The entire computational volume is free space with dimension $120 \times 120 \times 120$ uniform grid cells of size 20nm each. The TF region has dimension $100 \times 100 \times 100$ grid cells. The Mur ABC is used to terminate the computational volume. The simulation is performed over 1200 time steps of size $\Delta t = \frac{0.98\Delta}{c\sqrt{3}}$ each. The incident beam is propagating towards the $-z$ axis. The focal length of the lens is 10mm and the numerical aperture is $\sin\theta_{max} = 0.4$. The reference point is specified at the centre of the computational volume that is also the focal point of the lens. The source function $E_0(t)$ is modeled by a modulated Gaussian pulse in time: $\sin(\omega_0(t - t_0))e^{-(\frac{t-t_0}{\tau})^2}$ with $\tau = 112\Delta t$, $t_0 = 636\Delta t$ and $\omega_0 = 11.778\pi \times 10^{14}$ rad/s. The upper -40 dB magnitude of the source function spectrum corresponds to $N_\lambda = 20$. The integrations in (5.68) are numerically computed using the extended midpoint quadrature scheme [92], with a total number of 324 plane waves (accurately sourcing such a large number of plane waves by the 1-D grid based methods can be a challenging task).

Figs. 5.10(a)-(f) first plot the E_x field component (in dB) on the $y = 0$ (xz) plane at different time instants with the colorplot bar restricted to -40 dB. The E_x field is normalized by its maximum at the focal point. The white dotted-line represents the TF/SF boundary. Figs. 5.10(a)-(c) illustrate the beam entering the TF region and propagating towards the focal point. Fig. 5.10(d) shows the centre of the beam at the focal point at time step = 636. Figs. 5.10(e)-(f) illustrate the beam propagating away from the focal point and exiting the TF region. In all plots, the focused beam is well created and isolated in the TF region, using the proposed fields.

Figure 5.11: E_x scattered field leakage (in dB) comparison at grid point (61,61,10) on xy plane, 1 cell below the exit plane of the focused beam.

Next, we analyze the field leakage errors in the SF region. Figs. 5.11 and 5.12 plot the E_x scattered field leakage at the point (61,61,10) and (61,61,112), respectively, using the proposed fields and the field expressions without compensation and with the grid-velocity correction technique presented in [92]. The points (61,61,10) and (61,61,112) lie on the xy plane that is 1 cell below the exit plane and 1 cell above the entrance plane of the focused beam, respectively. Fig. 5.11 illustrates that the proposed field expressions achieves a maximum error level of -115.9 dB that is reduced by 87.04 dB and 67.8 dB from those without compensation and with the grid-velocity correction tech-

Figure 5.12: E_x scattered field leakage (in dB) comparison at grid point (61,61,112) on xy plane, 1 cell above the entrance plane of the focused beam.

nique, respectively. Similarly, Fig. 5.12 shows the proposed field expressions attaining a maximum error level that is reduced by 87.57 dB and 69.08 dB from those without compensation and with the grid-velocity correction technique, respectively. The reduction of error levels at the entrance and exit planes validate the higher-order compensations in the proposed fields.

5.7 Concluding Remarks

This chapter has presented an improved time-domain analytic method for accurately computing incident fields at the TF/SF boundary. Using analytic field expressions with higher-order dispersion and polarization compensations, the proposed method compensates for 1) the FDTD numerical dispersion; and 2) the lack of orthogonality between the frequency-dependent field polarizations and the wavevector, which was not accounted for in existing time-domain analytic methods. Formulations that facilitate the implementation of the proposed analytic expressions have also been presented.

Numerical experiments have been presented to demonstrate the proposed method's ability to source both 3-D plane wave and focused beam. From the experiments, it was shown that the proposed method is more accurate and can attain field leakage errors much lower than existing time-domain analytic methods. The proposed method is also practical as it can be used to compute the require incident fields at every time step, unlike the frequency-domain analytic methods that require additional memory to store the incident fields prior to the FDTD simulation.

These advantages make the proposed method a suitable analytic approach especially for introducing beam excitations (non-plane waves) into the TF/SF formulation. The higher-order compensations can potentially be used to develop accurate time-domain representations of other forms of incident beams or non-plane waves for the TF/SF formulation.

Chapter 6

Conclusion

In this thesis, we have developed FDTD methods for efficient and accurate modeling of EM interactions with complex media characterized by anisotropic constitutive relations. In particular, we have presented the extensions of implicit FDTD methods for anisotropic media as well as improving the accuracy of the time-domain analytic method in the Yee's FDTD TF/SF formulation.

In Chapter 3, we have presented a novel implicit split-step FDTD method for modeling 3-D wave propagation in general anisotropic media. An extension of the proposed method with PML boundary conditions was further exemplified. Stability analysis of the proposed split-step FDTD method using the Fourier method was presented. The eigenvalues of the Fourier amplification matrix were numerically shown to have unity magnitude even for time steps greater than the Courant-limit time step, thereby illustrating the stable and non-dissipative nature of the proposed split-step FDTD method in general anisotropic media. Five numerical experiments have been presented to further validate the stability, accuracy and efficiency of the proposed split-step FDTD method in general anisotropic media. It has been shown that the proposed split-step FDTD method

is generally more efficient compared to the explicit FDTD method when $CFLN \geq 4$. The proposed split-step FDTD method has also been shown to attain results that are in good agreement with the explicit FDTD method.

In Chapter 4, four extensions of the implicit CE-ADI-FDTD method were proposed for efficient modeling of anisotropic periodic structures. These four extensions were formulated using an efficient ADI splitting formulae. A CE-ADI-FDTD method was first generally formulated for inhomogeneous media composed of saturated ferrite with loss and anisotropic permittivity tensor. Auxiliary differential equation was used to model the saturated ferrite. This extension permitted the CE-ADI-FDTD method to analyze magnetic PhCs in addition to nonmagnetic PhCs. The CE-ADI-FDTD method was subsequently generally formulated for inhomogeneous media composed of anisotropic permittivity tensor and gain materials. Nonmagnetic PhCs with gain, such as laser dye doped cholesteric liquid crystals, can be efficiently analyzed using this extended CE-ADI-FDTD method. Circularly polarized lasing of a CLC was verified at the edge of the stop band. The conventional CE-ADI-FDTD formulation for nonmagnetic PhCs (without gain) was then presented in a more efficient form. A flops count and number of RHS terms comparison was made with the conventional CE-ADI-FDTD method, in which, it was noted that the proposed method has flops count and number of RHS terms reduced by about half times of those in the conventional method. Finally a 2-D extension of the CE-ADI-FDTD method was presented for inhomogeneous media with saturated ferrite. This extension can be used to efficiently analyze 2-D magnetic PhC structures. Numerical demonstration of the proposed CE-ADI-FDTD methods were presented using examples of both 1-D and 2-D magnetic and nonmagnetic PhCs. In the demonstration of nonmagnetic PhC, it was further highlighted that the field enhancement effect in the PhC can be optimized for an incident wave polarization by properly tuning the orientation angles of the anisotropy axes of the PhC layers. In general, the proposed methods

were shown to consume lesser computational time and fewer iterations while maintaining good agreement with existing results and the explicit FDTD as well as conventional CE-ADI-FDTD methods.

In Chapter 5, an improved time-domain analytic method was presented to accurately compute incident fields in the TF/SF formulation for FDTD scattering analysis of structures that can be anisotropic. The proposed method uses analytic expressions with higher-order dispersion and polarization compensations. Formulations that facilitate the implementation of the proposed method were also presented. Numerical experiments have been presented to demonstrate the proposed method's ability to source both 3-D plane wave and focused beam. From the experiments, it was shown that the proposed method is more accurate than existing methods and can attain field leakage errors as low as -115.9 dB, for a reasonably discretized grid. The proposed method is also practical as it can be used to compute the required incident fields at every time step, unlike the frequency-domain analytic methods that require additional memory to store the incident fields prior to the FDTD simulation.

Based on the research contributions, we present the following recommendations for future work:

- (1) Using the proposed splitting approach, further extensions of the implicit split-step FDTD method can be made to incorporate material loss and frequency dispersion. Such an implicit FDTD method can be quite useful to efficiently solve general problems with materials that are lossy, dispersive as well as anisotropic. In addition, the implicit split-step FDTD method can possibly be made more efficient by applying the fundamental splitting techniques with matrix-operator-free RHSs. Another future work is the possible parallelization of the implicit split-step FDTD

method for more efficient simulation of anisotropic media.

- (2) Following the procedures to attain the efficient CE-ADI-FDTD method, further extensions can potentially be made to model anisotropic periodic structures composed of materials that are both gyrotropic in permittivity and permeability [133]. In addition, the CE-ADI-FDTD method can potentially be extended to analyze 2-D and possibly 3-D wave propagation in anisotropic periodic structures, with and without gain.
- (3) Utilizing the presented higher-order compensations and additional formulations, it would be useful to derive accurate time-domain representations of other forms of focused beam and non-plane wave sources for the TF/SF formulation. Such non-plane waves could possibly include those of a dipole or infinite line source. Furthermore, following the presented procedures, one can possibly extend the time-domain analytic method to compute incident fields for implicit TF/SF FDTD methods. This would allow for efficient and accurate FDTD analysis of both plane and non-plane wave scattering from structures that can be anisotropic in nature.

Appendix A

Computation of Amplification Matrices

$\mathbf{G}_i$ and $\mathbf{G}$

The computation of amplification matrices $\mathbf{G}_i$ and $\mathbf{G}$ in Section 3.3 is as follows: Let $p_i^{r,c}$ and $q_i^{r,c}$ denote an element in row r and column c of 6×6 matrices $\mathbf{P}_i$ and $\mathbf{Q}_i$ respectively. Let $\theta_\alpha = \frac{k_\alpha \Delta \alpha}{2}$ with $\alpha = x, y$ and z . Except the following elements of matrices $\mathbf{P}_i$ and $\mathbf{Q}_i$, the remaining diagonal elements are unity and off-diagonal elements are zero:

$$\begin{aligned} q_1^{1,3} &= (-\kappa_{xz} \cos(\theta_x) \cos(\theta_z)) / \kappa_{zz} \\ q_1^{2,3} &= (-\kappa_{yz} \cos(\theta_y) \cos(\theta_z)) / \kappa_{zz} \\ q_1^{3,3} &= (1 - \frac{\Delta t^2}{\Delta x^2} \kappa_{zz} v_{yy} \sin^2(\theta_x)) / (1 + \frac{\Delta t^2}{\Delta x^2} \kappa_{zz} v_{yy} \sin^2(\theta_x)) \\ q_1^{5,3} &= -j \frac{\Delta t}{\Delta x} v_{yy} \sin(\theta_x) \\ q_1^{3,5} &= (-j 2 \frac{\Delta t}{\Delta x} \kappa_{zz} \sin(\theta_x)) / (1 + \frac{\Delta t^2}{\Delta x^2} \kappa_{zz} v_{yy} \sin^2(\theta_x)) \\ q_1^{4,5} &= (-v_{xy} \cos(\theta_x) \cos(\theta_y)) / v_{yy} \\ q_1^{6,5} &= (-v_{zy} \cos(\theta_y) \cos(\theta_z)) / v_{yy} \end{aligned}$$

$$p_1^{1,3} = q_1^{1,3} \quad p_1^{2,3} = q_1^{2,3} \quad p_1^{5,3} = -q_1^{5,3}$$

$$p_1^{4,5} = q_1^{4,5} \quad p_1^{6,5} = q_1^{6,5}$$

$$q_2^{1,1} = (1 - \frac{\Delta t^2}{\Delta y^2} \kappa_{xx} v_{zz} \sin^2(\theta_y)) / (1 + \frac{\Delta t^2}{\Delta y^2} \kappa_{xx} v_{zz} \sin^2(\theta_y))$$

$$q_2^{2,1} = (-\kappa_{yx} \cos(\theta_x) \cos(\theta_y)) / \kappa_{xx}$$

$$q_2^{3,1} = (-\kappa_{zx} \cos(\theta_x) \cos(\theta_z)) / \kappa_{xx}$$

$$q_2^{6,1} = -j \frac{\Delta t}{\Delta y} v_{zz} \sin(\theta_y)$$

$$q_2^{1,6} = (-j 2 \frac{\Delta t}{\Delta y} \kappa_{xx} \sin(\theta_y)) / (1 + \frac{\Delta t^2}{\Delta y^2} \kappa_{xx} v_{zz} \sin^2(\theta_y))$$

$$q_2^{4,6} = (-v_{xz} \cos(\theta_x) \cos(\theta_z)) / v_{zz}$$

$$q_2^{5,6} = (-v_{yz} \cos(\theta_y) \cos(\theta_z)) / v_{zz}$$

$$p_2^{2,1} = q_2^{2,1} \quad p_2^{3,1} = q_2^{3,1} \quad p_2^{6,1} = -q_2^{6,1}$$

$$p_2^{4,6} = q_2^{4,6} \quad p_2^{5,6} = q_2^{5,6}$$

$$q_3^{1,2} = (-\kappa_{xy} \cos(\theta_x) \cos(\theta_y)) / \kappa_{yy}$$

$$q_3^{2,2} = (1 - \frac{\Delta t^2}{\Delta z^2} \kappa_{yy} v_{xx} \sin^2(\theta_z)) / (1 + \frac{\Delta t^2}{\Delta z^2} \kappa_{yy} v_{xx} \sin^2(\theta_z))$$

$$q_3^{3,2} = (-\kappa_{zy} \cos(\theta_y) \cos(\theta_z)) / \kappa_{yy}$$

$$q_3^{4,2} = -j \frac{\Delta t}{\Delta z} v_{xx} \sin(\theta_z)$$

$$q_3^{2,4} = (-j 2 \frac{\Delta t}{\Delta z} \kappa_{yy} \sin(\theta_z)) / (1 + \frac{\Delta t^2}{\Delta z^2} \kappa_{yy} v_{xx} \sin^2(\theta_z))$$

$$q_3^{5,4} = (-v_{yx} \cos(\theta_x) \cos(\theta_y)) / v_{xx}$$

$$q_3^{6,4} = (-v_{zx} \cos(\theta_x) \cos(\theta_z)) / v_{xx}$$

$$p_3^{1,2} = q_3^{1,2} \quad p_3^{3,2} = q_3^{3,2} \quad p_3^{4,2} = -q_3^{4,2}$$

$$p_3^{5,4} = q_3^{5,4} \quad p_3^{6,4} = q_3^{6,4}$$

$$\begin{aligned}
q_4^{1,2} &= (-\kappa_{xy} \cos(\theta_x) \cos(\theta_y)) / \kappa_{yy} \\
q_4^{2,2} &= (1 - \frac{\Delta t^2}{\Delta x^2} \kappa_{yy} v_{zz} \sin^2(\theta_x)) / (1 + \frac{\Delta t^2}{\Delta x^2} \kappa_{yy} v_{zz} \sin^2(\theta_x)) \\
q_4^{3,2} &= (-\kappa_{zy} \cos(\theta_y) \cos(\theta_z)) / \kappa_{yy} \\
q_4^{6,2} &= j \frac{\Delta t}{\Delta x} v_{zz} \sin(\theta_x) \\
q_4^{2,6} &= (j 2 \frac{\Delta t}{\Delta x} \kappa_{yy} \sin(\theta_x)) / (1 + \frac{\Delta t^2}{\Delta x^2} \kappa_{yy} v_{zz} \sin^2(\theta_x)) \\
q_4^{4,6} &= (-v_{xz} \cos(\theta_x) \cos(\theta_z)) / v_{zz} \\
q_4^{5,6} &= (-v_{yz} \cos(\theta_y) \cos(\theta_z)) / v_{zz} \\
p_4^{1,2} &= q_4^{1,2} \quad p_4^{3,2} = q_4^{3,2} \quad p_4^{6,2} = -q_4^{6,2} \\
p_4^{4,6} &= q_4^{4,6} \quad p_4^{5,6} = q_4^{5,6}
\end{aligned}$$

$$\begin{aligned}
q_5^{1,3} &= (-\kappa_{xz} \cos(\theta_x) \cos(\theta_z)) / \kappa_{zz} \\
q_5^{2,3} &= (-\kappa_{yz} \cos(\theta_y) \cos(\theta_z)) / \kappa_{zz} \\
q_5^{3,3} &= (1 - \frac{\Delta t^2}{\Delta y^2} \kappa_{zz} v_{xx} \sin^2(\theta_y)) / (1 + \frac{\Delta t^2}{\Delta y^2} \kappa_{zz} v_{xx} \sin^2(\theta_y)) \\
q_5^{4,3} &= j \frac{\Delta t}{\Delta y} v_{xx} \sin(\theta_y) \\
q_5^{3,4} &= (j 2 \frac{\Delta t}{\Delta y} \kappa_{zz} \sin(\theta_y)) / (1 + \frac{\Delta t^2}{\Delta y^2} \kappa_{zz} v_{xx} \sin^2(\theta_y)) \\
q_5^{5,4} &= (-v_{yx} \cos(\theta_x) \cos(\theta_y)) / v_{xx} \\
q_5^{6,4} &= (-v_{zx} \cos(\theta_x) \cos(\theta_z)) / v_{xx} \\
p_5^{1,3} &= q_5^{1,3} \quad p_5^{2,3} = q_5^{2,3} \quad p_5^{4,3} = -q_5^{4,3} \\
p_5^{5,4} &= q_5^{5,4} \quad p_5^{6,4} = q_5^{6,4}
\end{aligned}$$

$$q_6^{1,1} = (1 - \frac{\Delta t^2}{\Delta z^2} \kappa_{xx} v_{yy} \sin^2(\theta_z)) / (1 + \frac{\Delta t^2}{\Delta z^2} \kappa_{xx} v_{yy} \sin^2(\theta_z))$$

$$q_6^{2,1} = (-\kappa_{yx} \cos(\theta_x) \cos(\theta_y)) / \kappa_{xx}$$

$$q_6^{3,1} = (-\kappa_{zx} \cos(\theta_x) \cos(\theta_z)) / \kappa_{xx}$$

$$q_6^{5,1} = j \frac{\Delta t}{\Delta z} v_{yy} \sin(\theta_z)$$

$$q_6^{1,5} = (j 2 \frac{\Delta t}{\Delta z} \kappa_{xx} \sin(\theta_z)) / (1 + \frac{\Delta t^2}{\Delta z^2} \kappa_{xx} v_{yy} \sin^2(\theta_z))$$

$$q_6^{4,5} = (-v_{xy} \cos(\theta_x) \cos(\theta_y)) / v_{yy}$$

$$q_6^{6,5} = (-v_{zy} \cos(\theta_y) \cos(\theta_z)) / v_{yy}$$

$$p_6^{2,1} = q_6^{2,1} \quad p_6^{3,1} = q_6^{3,1} \quad p_6^{5,1} = -q_6^{5,1}$$

$$p_6^{4,5} = q_6^{4,5} \quad p_6^{6,5} = q_6^{6,5}.$$

The amplification matrix $\mathbf{G}_i$ and $\mathbf{G}$ can then be determined using $\mathbf{G}_i = \mathbf{P}_i^{-1} \mathbf{Q}_i$ and $\mathbf{G} = \mathbf{G}_6 \mathbf{G}_5 \mathbf{G}_4 \mathbf{G}_3 \mathbf{G}_2 \mathbf{G}_1$.

Appendix B

Coefficients $c_{2,4}^{t,p}$ and $s_{2,4}^{t,p}$

The coefficients $c_{2,4}^{t,p}$ and $s_{2,4}^{t,p}$ in Section 5.3.2 are as follows:

$$\begin{aligned}
 c_2^t &= \sin^2 \theta \alpha_2^z & c_4^t &= \sin^2 \theta \alpha_4^z \\
 s_2^t &= -\cos^2 \theta \alpha_2^z & s_4^t &= -\cos^2 \theta \left(\frac{\alpha_2^{z^2}}{2} + \alpha_4^z \right) \\
 c_2^p &= \cos^2 \theta \alpha_2^z + \alpha_2^x & c_4^p &= \cos^2 \theta \left(\frac{\sin^2 \theta}{2} \alpha_2^{z^2} + \beta^x \right) + \alpha_4^x \\
 s_2^p &= \cos^2 \theta \alpha_2^z + \alpha_2^y & s_4^p &= \cos^2 \theta \left(\frac{\sin^2 \theta}{2} \alpha_2^{z^2} + \beta^y \right) + \alpha_4^y
 \end{aligned}$$

in which

$$\begin{aligned}
 \alpha_2^x &= \frac{1}{24} \left(\frac{P_2}{c^2 \Delta t^2} - \frac{\Delta x^2 \cos^2 \phi \sin^2 \theta}{c^2 \Delta t^2} \right) \\
 \alpha_2^y &= \frac{1}{24} \left(\frac{P_2}{c^2 \Delta t^2} - \frac{\Delta y^2 \sin^2 \phi \sin^2 \theta}{c^2 \Delta t^2} \right)
 \end{aligned}$$

$$\begin{aligned}
\alpha_2^z &= \frac{1}{24} \frac{P_2^s}{c^2 \Delta t^2} \\
\alpha_4^x &= \left(\frac{P_2}{c^2 \Delta t^2} - \frac{1}{2} \right) \frac{\alpha_2^x}{6} - \frac{\alpha_2^{x^2}}{2} - \frac{1}{720} \left(\frac{P_4}{c^4 \Delta t^4} - \frac{\Delta x^4 \cos^4 \phi \sin^4 \theta}{c^4 \Delta t^4} \right) \\
\alpha_4^y &= \left(\frac{P_2}{c^2 \Delta t^2} - \frac{1}{2} \right) \frac{\alpha_2^y}{6} - \frac{\alpha_2^{y^2}}{2} - \frac{1}{720} \left(\frac{P_4}{c^4 \Delta t^4} - \frac{\Delta y^4 \sin^4 \phi \sin^4 \theta}{c^4 \Delta t^4} \right) \\
\alpha_4^z &= \left(\frac{P_2}{c^2 \Delta t^2} - \frac{1}{2} \right) \frac{\alpha_2^z}{6} - \frac{\alpha_2^{z^2}}{2} \sin^2 \theta - \frac{1}{720} \frac{P_4^s}{c^4 \Delta t^4} \\
\beta^x &= \frac{3}{2} \cos^2 \theta \alpha_2^{z^2} + \alpha_2^x \alpha_2^z + \alpha_4^z \\
\beta^y &= \frac{3}{2} \cos^2 \theta \alpha_2^{z^2} + \alpha_2^y \alpha_2^z + \alpha_4^z \\
P_2^s &= \Delta x^2 \cos^4 \phi \sin^2 \theta + \Delta y^2 \sin^4 \phi \sin^2 \theta - \Delta z^2 \cos^2 \theta \\
P_4^s &= \Delta x^4 \cos^6 \phi \sin^4 \theta + \Delta y^4 \sin^6 \phi \sin^4 \theta - \Delta z^4 \cos^4 \theta.
\end{aligned}$$

Note that P_2 and P_4 are given in Section 5.3.1.

Appendix C

Coefficients $\Delta U_{E,2}$ and $\Delta U_{E,4}$ for Plane Wave Excitation

The coefficients $\Delta U_{E,2}$ and $\Delta U_{E,4}$ for plane wave excitation in Sections 5.3.2 and 5.3.3 are as follows:

$$\begin{aligned} \Delta U_{E,2} &= \begin{bmatrix} U_{Ex}^a(\cos^2 \theta \alpha_2^z + \alpha_2^y) + U_{Ex}^b(\alpha_2^z + \alpha_2^x) \\ U_{Ey}^a(\cos^2 \theta \alpha_2^z + \alpha_2^x) + U_{Ey}^b(\alpha_2^z + \alpha_2^y) \\ U_{Ez}^a \cos^2 \theta \alpha_2^z \end{bmatrix} \end{aligned}$$

$$\begin{aligned} \Delta U_{E,4} &= \begin{bmatrix} U_{Ex}^a(\cos^2 \theta (\frac{\sin^2 \theta}{2} \alpha_2^{z2} + \beta^y) + \alpha_4^y) + U_{Ex}^b(\beta^x + \alpha_4^x) \\ U_{Ey}^a(\cos^2 \theta (\frac{\sin^2 \theta}{2} \alpha_2^{z2} + \beta^x) + \alpha_4^x) + U_{Ey}^b(\beta^y + \alpha_4^y) \\ U_{Ez}^a \cos^2 \theta (\frac{\alpha_2^{z2}}{2} + \alpha_4^z) \end{bmatrix} \end{aligned}$$

with α and β coefficients given in Appendix B and

$$U_{Ex}^a = \cos \psi \sin \phi$$

$$U_{Ex}^b = -\sin \psi \cos \theta \cos \phi$$

$$U_{Ey}^a = -\cos \psi \cos \phi$$

$$U_{Ey}^b = -\sin \psi \cos \theta \sin \phi$$

$$U_{Ez}^a = -\sin \psi \sin \theta.$$

Appendix D

Coefficients $\Delta U_{E,2}$ and $\Delta U_{E,4}$ for Focused Beam Excitation

The coefficients $\Delta U_{E,2}$ and $\Delta U_{E,4}$ for focused beam excitation in Section 5.3.4 are as follows:

$$\Delta U_{E,2} = \begin{bmatrix} \cos^2 \phi \cos \theta (c_2^t + 2c_2^p) + 2\sin^2 \phi s_2^p \\ \sin \phi \cos \phi ((\cos \theta - 1)(c_2^p + s_2^p) + \cos \theta c_2^t) \\ -\alpha_2^x \cos \phi \sin \theta \end{bmatrix}$$
$$\Delta U_{E,4} = \begin{bmatrix} \cos^2 \phi \cos \theta (c_4^t + c_2^{p2} + 2c_2^p c_2^t + 2c_4^p) + \sin^2 \phi (s_2^{p2} + 2s_4^p) \\ \sin \phi \cos \phi ((\cos \theta - 1)(c_4^p + s_2^p c_2^p + s_4^p) + \cos \theta (c_2^t c_2^p + c_2^t s_2^p + c_4^t)) \\ -\alpha_4^x \cos \phi \sin \theta \end{bmatrix}$$

where coefficients $c_{2,4}^{t,p}$ and $s_{2,4}^{t,p}$ are presented in Appendix B.

Appendix E

Derivation of Recurrence Relations for $g_n^s(t)$ and $g_n^c(t)$

The derivation of recurrence relations for $g_n^s(t)$ and $g_n^c(t)$ in Section 5.4 are as follows:

From (5.73), the $n + 1$ derivative of $g(t)$ can be expressed as

$$\frac{d^{n+1}}{dt^{n+1}}g(t) = \left(\frac{-1}{\tau}\right)^{n+1}e^{-\left(\frac{t}{\tau}\right)^2}(\sin(\omega_0 t)g_{n+1}^s(t) + \cos(\omega_0 t)g_{n+1}^c(t)). \quad (\text{E.1})$$

The $n + 1$ derivative of $g(t)$ can also be attained by taking the derivative of $\frac{d^n}{dt^n}g(t)$ as

$$\begin{aligned} \frac{d}{dt}\left(\frac{d^n}{dt^n}g(t)\right) &= \left(\frac{-1}{\tau}\right)^{n+1}e^{-\left(\frac{t}{\tau}\right)^2}[\sin(\omega_0 t)\left(\frac{2t}{\tau}g_n^s(t) - \tau\frac{d}{dt}g_n^s(t) + \omega_0\tau g_n^c(t)\right) \\ &\quad + \cos(\omega_0 t)\left(\frac{2t}{\tau}g_n^c(t) - \tau\frac{d}{dt}g_n^c(t) - \omega_0\tau g_n^s(t)\right)]. \quad (\text{E.2}) \end{aligned}$$

By comparing (E.1) and (E.2), it can be noted that

$$g_{n+1}^s(t) = \frac{2t}{\tau} g_n^s(t) - \tau \frac{d}{dt} g_n^s(t) + \omega_0 \tau g_n^c(t) \quad (\text{E.3})$$

$$g_{n+1}^c(t) = \frac{2t}{\tau} g_n^c(t) - \tau \frac{d}{dt} g_n^c(t) - \omega_0 \tau g_n^s(t). \quad (\text{E.4})$$

In (E.3)-(E.4), $\frac{d}{dt} g_n^s(t)$ and $\frac{d}{dt} g_n^c(t)$ can be expressed in terms of their respective past values. Consider when n is even. From (5.74),

$$\begin{aligned} \frac{d}{dt} g_n^s(t) &= \frac{d}{dt} \sum_{r=0}^n \binom{n}{r} (-1)^{\frac{r}{2}} (\omega_0 \tau)^r H_{n-r}\left(\frac{t}{\tau}\right) \\ &= \frac{d}{dt} \left[\sum_{r=0}^{n-2} \binom{n}{r} (-1)^{\frac{r}{2}} (\omega_0 \tau)^r H_{n-r}\left(\frac{t}{\tau}\right) + \binom{n}{n} (-1)^{\frac{n}{2}} (\omega_0 \tau)^n H_0\left(\frac{t}{\tau}\right) \right] \\ &= \sum_{r=0}^{n-2} \binom{n}{r} (-1)^{\frac{r}{2}} (\omega_0 \tau)^r \frac{d}{dt} H_{n-r}\left(\frac{t}{\tau}\right). \end{aligned} \quad (\text{E.5})$$

Using the relation $\frac{d}{dt} H_n\left(\frac{t}{\tau}\right) = \frac{2n}{\tau} H_{n-1}\left(\frac{t}{\tau}\right)$ in (E.5) yields

$$\frac{d}{dt} g_n^s(t) = \frac{1}{\tau} \sum_{r=0}^{n-2} \binom{n}{r} (-1)^{\frac{r}{2}} (\omega_0 \tau)^r 2(n-r) H_{n-r-1}\left(\frac{t}{\tau}\right). \quad (\text{E.6})$$

Using the identity $(n-r) \binom{n}{r} = n \binom{n-1}{r}$ in (E.6) finally gives

$$\begin{aligned} \frac{d}{dt} g_n^s(t) &= \frac{2n}{\tau} \sum_{r=0}^{n-2} \binom{n-1}{r} (-1)^{\frac{r}{2}} (\omega_0 \tau)^r H_{n-r-1}\left(\frac{t}{\tau}\right) \\ &= \frac{2n}{\tau} g_{n-1}^s(t). \end{aligned} \quad (\text{E.7})$$

Hence, from (E.7), we have expressed $\frac{d}{dt}g_n^s(t)$ in terms of its past value. The same expression is attained when n is odd. Following the derivations (E.5)-(E.7), the expression for $\frac{d}{dt}g_n^c(t) = \frac{2n}{\tau}g_{n-1}^c(t)$ can also be attained when n is both even and odd.

Substitution of $\frac{d}{dt}g_n^s(t) = \frac{2n}{\tau}g_{n-1}^s(t)$ and $\frac{d}{dt}g_n^c(t) = \frac{2n}{\tau}g_{n-1}^c(t)$ into (E.3) and (E.4), respectively, and setting $n = n - 1$ finally gives the recurrence relations

$$\begin{aligned} g_n^s(t) &= \frac{2t}{\tau}g_{n-1}^s(t) - 2(n-1)g_{n-2}^s(t) + \omega_0\tau g_{n-1}^c(t) \\ g_n^c(t) &= \frac{2t}{\tau}g_{n-1}^c(t) - 2(n-1)g_{n-2}^c(t) - \omega_0\tau g_{n-1}^s(t). \end{aligned}$$

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Author's Publications

Journal Publications:

1. G. Singh, E. L. Tan, Z. N. Chen, "Split-step finite-difference time-domain method with perfectly matched layers for efficient analysis of two-dimensional photonic crystals with anisotropic media," *Opt. Lett.*, vol. 37, no. 3, pp. 326-328, Feb. 2012.
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Conference Publications:

1. G. Singh, E. L. Tan, Z. N. Chen, “Analytic fields of a focused beam with higher-order compensations for FDTD TF/SF formulation,” *Proc. IEEE Antennas Propagat. Soc. Int. Symp.*, 2011.
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