Finite-difference time-domain methods for lossy and dispersive media

Heh, Ding Yu

2012

Heh, D. Y. (2012). Finite-difference time-domain methods for lossy and dispersive media.
Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/50621>

<https://doi.org/10.32657/10356/50621>

FINITE-DIFFERENCE TIME-DOMAIN METHODS FOR LOSSY AND DISPERSIVE MEDIA

HEH DING YU

School of Electrical and Electronic Engineering

A thesis submitted to the Nanyang Technological University
in partial fulfilment of the requirement for the degree of
Doctor of Philosophy

2012

Acknowledgements

First and foremost, I am greatly indebted to my supervisor, Assoc. Prof. Tan Eng Leong for his guidance throughout my Ph.D. candidature. His valuable advice and suggestions have contributed towards the success of this thesis. I am also grateful for his help and support which have kept me motivated at all times.

I would like to thank the faculty and laboratory staffs at the School of Electrical and Electronic Engineering for their support and assistance. I would also like to thank Nanyang Technological University, Singapore for all the research facilities and scholarships provided.

Last but not least, special thanks to my parents and family members for their love and support. Also, thanks to fellow friends who have made my learning journey a memorable one.

Table of Contents

Acknowledgements	i
Abstract	vii
List of Abbreviations and Symbols	ix
List of Figures	xii
List of Tables	xvii
1 Introduction	1
1.1 Motivation	1
1.2 Objectives	3
1.3 Major Contributions	3
1.4 Organization of the Thesis	6
2 A Brief Literature Survey on FDTD Methods	9
2.1 Maxwell's Equations	9
2.1.1 Lossy Media	12
2.1.2 Dispersive Media	14
2.2 Yee's Explicit FDTD Method	16
2.2.1 For Lossy Media	16
2.2.2 Extensions to Dispersive Media	18
2.3 ADI-FDTD Method	31

2.3.1	For Lossy Media	31
2.3.2	Extensions to Dispersive Media	35
2.4	Stability and Dispersion Analysis	38
3	Yee's Explicit FDTD Method for Lossy and Dispersive Media	42
3.1	Introduction	42
3.2	Yee's Explicit FDTD Schemes for Doubly Lossy Media	45
3.3	Generalized Stability Criterion for Doubly Lossy Media	47
3.4	Numerical Results for Stability Analysis	51
3.5	Dispersion Analysis for Doubly Lossy Media	56
3.5.1	Resolving Both Wavelength and Skin Depth	57
3.5.2	3-D Dispersion Analysis	59
3.5.3	Numerical Simulation	64
3.6	Z-Transform and Corrected Impulse Invariance	67
3.7	Formulations for Debye Dispersive Media	72
3.7.1	Formulation from D and E Relation	73
3.7.2	Formulation from P and E Relation	74
3.7.3	Formulation from J and E Relation	76
3.7.4	Memory Storage Requirements	77
3.8	Formulations For Lorentz Dispersive Media	78
3.8.1	Formulation from D and E Relation	78
3.8.2	Formulation from P and E Relation	80
3.8.3	Formulation for J and E Relation	81
3.8.4	Memory Storage Requirements	82
3.9	Dispersion Relation and Complex Numerical Permittivity	83
3.10	Numerical Results for Corrected Impulse Invariance	87
3.11	Conclusions	92
4	Unconditionally Stable FADI-FDTD Method for Lossy and Dispersive Media	94

4.1	Introduction	94
4.2	Generalized Lyapunov Stability Analysis	97
4.3	Generalized Matrix Norm Stability Analysis	102
4.4	Stability Analysis of Various ADI-FDTD Schemes for Doubly Lossy Media	104
4.4.1	Averaging	104
4.4.2	Forward-Backward	105
4.4.3	Backward-Forward	106
4.4.4	Exponential Time Differencing	107
4.4.5	Forward-Forward	109
4.4.6	Backward-Backward	110
4.4.7	Lossless	112
4.5	Von Neumann Method	113
4.6	Unifications of Source-Incorporated ADI-FDTD Schemes for Doubly Lossy Media	115
4.6.1	Unified Conventional Form (With RHS Matrix-Operators)	115
4.6.2	Unified Efficient Fundamental Form (With RHS Matrix-Operator-Free)	118
4.7	Implementation of Unified Efficient FADI-FDTD Schemes	119
4.7.1	Unified Update Equations	119
4.7.2	Field Memory Arrays	124
4.7.3	Parameter Memory Arrays	125
4.7.4	PEC and PMC Implementations	126
4.8	Numerical Results	127
4.8.1	CPU Time Saving	127
4.8.2	Numerical Examples for PEC and PMC Implementations	128
4.8.3	Asymmetry and Numerical Errors	130
4.8.4	Specific Absorption Rate (SAR)	135
4.9	FADI-FDTD Formulation for Various Dispersive Media Models	139
4.9.1	Generalized Formulation	139

4.9.2	Complex Conjugate Pole-Residue Pair	152
4.9.3	Debye	153
4.9.4	Lorentz	155
4.9.5	Drude	156
4.10	Conclusions	157
5	Applications of FADI-FDTD Method for Lossy and Dispersive Media	159
5.1	Introduction	159
5.2	Modeling Reverberation Chamber in Mode-Stirred Operation	160
5.2.1	Time Variant Conductivity Model for Reverberation Chamber in Mode-Stirred Operation	161
5.2.2	Numerical Results	161
5.3	Modeling Hemoglobin at Optical Frequency Using FADI-FDTD Method	165
5.3.1	Complex Relative Permittivity Model for Hemoglobin	166
5.3.2	Numerical Results	171
5.4	Modeling the Interaction of Terahertz Pulse with Healthy Skin and Basal Cell Carcinoma (BCC) Using FADI-FDTD Method	179
5.4.1	Complex Relative Permittivity Model for Human Skin	180
5.4.2	Reflected terahertz pulse	181
5.4.3	BCC detection based on reflected terahertz pulse	183
5.5	Analysis of Optical Waveguide Using FADI-FDTD Method	194
5.5.1	Complex Relative Permittivity Model for Metal	195
5.5.2	Numerical Results	198
5.6	Conclusions	208
6	Conclusions and Future Work	209
6.1	Conclusions	209
6.2	Suggestions for Future Work	213
	Author's Publications	215

Bibliography	217
---------------------	------------

Abstract

The finite-difference time-domain (FDTD) method has been widely used for solving various electromagnetic problems involving electromagnetic radiation, propagation and scattering. This thesis presents the analysis and applications of FDTD methods for lossy and dispersive media. The stability analysis is first performed on Yee's explicit FDTD schemes for doubly lossy media whereby a generalized stability criterion applicable for all 3-D explicit FDTD schemes is found. Similarly, the 3-D dispersion analysis reveals some important dispersion characteristics of 3-D explicit FDTD schemes for doubly lossy media. The thesis next proposes a corrected impulse invariance method as the current classical impulse invariance method used in explicit FDTD for dispersive media is found to be inaccurate. A corrected Z-transform table is provided to facilitate the conversion from frequency to Z domain. With the aid of the table, various formulations of FDTD update equations can be carried out conveniently.

For unconditionally stable alternating-direction-implicit FDTD (ADI-FDTD) method, Lyapunov and matrix norm stability analysis is applied on various ADI schemes for doubly lossy media. A rigorous analytical proof of unconditional stability is provided. Subsequently, a unified efficient fundamental ADI-FDTD (FADI-FDTD) schemes for lossy media is formulated. They are formulated in the *simplest*, *most concise*, *most efficient*, and *most fundamental* form of ADI-FDTD. Such efficient fundamental schemes have substantially less right-hand-side (RHS) update coeffi-

cients and field variables compared to the conventional ADI-FDTD schemes. Thus, they feature higher efficiency with reduced memory indexing and arithmetic operations. Further, the generalized formulation of FADI-FDTD method for dispersive media is provided. It is efficient, robust and applicable to Debye, Lorentz, Drude and complex conjugate pole-residue pair models.

Finally, the applications of FADI-FDTD method in the areas of electromagnetic compatibility, bioelectromagnetics and photonics are demonstrated. In electromagnetic compatibility, the modeling of reverberation chamber in mode-stirred operation is presented. A time variant complex relative permittivity is introduced such that the boundary conditions inside the chamber can be altered continuously for mode-stirred operation. For application in bioelectromagnetics, the interaction of light with hemoglobin at optical frequency is presented. An accurate model based on complex conjugate pole-residue pair is proposed to model the complex permittivity of hemoglobin at optical frequency. The interaction of terahertz pulse with healthy skin and basal cell carcinoma (BCC) is then demonstrated, where the human skin is modeled as Debye media. For application in photonics, the characteristics of a optical waveguide with Au (gold) and Ag (silver) metal cladding, modeled as combination of Drude-Lorentz dispersive media is analyzed. Further analysis of plasmonic waveguide grating filter is also shown.

List of Abbreviations and Symbols

Abbreviations

ADE	auxiliary differential equation
ADI	alternating-direction-implicit
BCC	basal cell carcinoma
CFL	Courant-Friedrich-Lewy
CFLN	Courant-Friedrich-Lewy number
CN	Crank-Nicholson
CPU	central processing unit
CPW	cell per wavelength
ETD	exponential-time-differencing
FADI	fundamental alternating-direction-implicit
FDTD	finite-difference time-domain
GPU	graphic processing unit
LHS	left-hand-side
LOD	locally-one-dimensional
MMS	Mohs micrographic surgery
PEC	perfect electric conductor
PLRC	piecewise linear recursive convolution
PMC	perfect magnetic conductor
PML	perfectly matched layer
RC	recursive convolution
RHS	right-hand-side

SAR	specific absorption rate
TA	time-average
TB	time-backward
TE	transverse electric
TF	time-forward
TF/SF	total-field/scattered-field
THz	terahertz
TM	transverse magnetic

Symbols

E_x, E_y, E_z	electric field components
H_x, H_y, H_z	magnetic field components
t, f, ω	time, frequency, angular frequency
$\Delta x, \Delta y, \Delta z, \Delta t$	spatial and time steps
$\epsilon, \epsilon_0, \epsilon_r$	permittivity, free space permittivity, relative permittivity
μ, μ_0, μ_r	permeability, free space permeability, relative permeability
σ, σ^*	electric and magnetic conductivities
$\epsilon_\infty, \mu_\infty$	permittivity and permeability at infinite frequency
a_p, b_p	p -th electric and magnetic poles
r_p, q_p	p -th electric and magnetic residues
$\Delta\epsilon_p, \Delta\mu_p$	change in relative permittivity and permeability of p -th dispersive pole
$\tau_p, \tau_{e,p}, \tau_{h,p}$	electric and magnetic relaxation times of p -th Debye pole
$\omega_p, \omega_{e,p}, \omega_{h,p}$	electric and magnetic resonant frequencies of p -th Lorentz or Drude pole
$\delta_p, \delta_{e,p}, \delta_{h,p}$	electric and magnetic damping coefficients of p -th Lorentz pole

$\nu_p, \nu_{e,p}, \nu_{h,p}$	electric and magnetic inverse relaxation times of p -th Drude pole
-------------------------------	--

List of Figures

3.1	3-D plots of stability factor with respect to $\sigma/\omega\epsilon$ and $\sigma^*/\omega\mu$ for (a) TA, (b) ETD, (c) TF, (d) TB. ©2010 IEEE.	52
3.2	Snapshot of reflected and transmitted electric fields through thin conductor ($\sigma = 10^5\text{S/m}$, $\sigma^* = 10^5\Omega/\text{m}$) after 96.5ps. ©2010 IEEE. . . .	53
3.3	Instability shown by TA around thin conductor after 1000 iterations (Δt set at maximum allowed Δt of ETD instead of its own). ©2010 IEEE.	54
3.4	(a) Phase velocity and (b) attenuation errors with respect to $\sigma/\omega\epsilon$. $\sigma^*/\omega\mu = 10^{-2}$, CPW=40.	58
3.5	Phase velocity error for (a) ETD, (b) TA, (c) TF and (d) TB with respect to θ and ϕ . $\sigma/\omega\epsilon = \sigma^*/\omega\mu = 10^2$, $N=10$	60
3.6	Positive and negative maximum (a) phase velocity and (b) attenuation errors with respect to $\sigma/\omega\epsilon$. $\sigma^*/\omega\mu = 10^{-2}$, $N=40$. Dash lines represent negative maximum errors.	62
3.7	Same as Fig. 3.6, but for $\sigma^*/\omega\mu = 10^0$	63
3.8	Same as Fig. 3.6, but for $\sigma^*/\omega\mu = 10^2$	64
3.9	Positive and negative maximum (a) phase velocity and (b) attenuation errors with respect to frequency. No negative maximum errors here. $\sigma = 60\text{S/m}$, $\sigma^* = 800\Omega/\text{m}$, $N = 10$ at $f_{max} = 10\text{GHz}$	65
3.10	Same as Fig. 3.9, but for $N = 40$. Dash lines represent negative maximum errors.	66
3.11	(a) Phase velocity and (b) attenuation anisotropy errors with respect to $\sigma/\omega\epsilon$. $\sigma^*/\omega\mu = 10^{-2}$, $N = 40$	67
3.12	Same as Fig. 3.11, but for $\sigma^*/\omega\mu = 10^0$	68
3.13	Same as Fig. 3.11, but for $\sigma^*/\omega\mu = 10^2$	69

3.14	Normalized absolute electric field error with respect to (a) cell position for 1-D problem and (b) time for 3-D problem in a doubly lossy medium. $N = 10$	70
3.15	Normalized (a) phase and (b) attenuation errors versus frequency using various formulations for Debye media. ©2009 IEEE.	87
3.16	Normalized (a) phase and (b) attenuation errors versus frequency using various formulations for Lorentz media.	88
3.17	Absolute electric field error versus cell position computed using various formulations of (a) classical and (b) corrected impulse invariance methods for Debye media. ©2009 IEEE.	90
3.18	Absolute electric field error versus cell position computed using various formulations of (a) JE and (b) DE_{cor} , DE , PE_{cor} , PE , ADE and PLRC methods for Lorentz media.	91
4.1	Normalized electric field leakage recorded at the centre of PEC sphere using different schemes. Only forward-backward scheme exhibits electric field leakage.	130
4.2	Same as Fig. 4.1, but for PMC sphere. Again, only forward-forward scheme exhibits electric field leakage.	131
4.3	Asymmetry error (in dB) with respect to x and y grid positions for (a) exponential time differencing, (b) averaging, (c) forward-forward and (d) forward-backward schemes. Forward-backward scheme records considerably higher electric field asymmetry error.	132
4.4	Normalized electric field error exhibited by various schemes for (a) CFLN=5 and (b) CFLN=10.	133
4.5	Magnitude of reflection coefficient for a half space lossy medium computed using various schemes.	134
4.6	SAR of human skin at 42.25 GHz with respect to depth and width. .	137
4.7	SAR of human skin at 61.22 GHz with respect to depth and width. .	137
4.8	SAR of human skin at 42.25 GHz and 61.22 GHz with respect to depth.	138
4.9	Normalized SAR error with respect to depth and width at 42.25 GHz for ETD scheme.	139
4.10	Normalized SAR error with respect to depth and width at 42.25 GHz for averaging scheme.	140
4.11	Normalized SAR error with respect to depth and width at 42.25 GHz for forward-forward scheme.	141

5.1	Magnitude of electric field components at 200 MHz along a line. . . .	162
5.2	Same as Fig. 5.1, but for reverberation chamber with stationary stirrer.	163
5.3	Standard deviation (in dB) of electric field components with respect to frequency.	164
5.4	Same as Fig. 5.3, but for reverberation chamber with stationary stirrer.	165
5.5	(a) Real part of complex refractive index, n_r and (b) extinction coefficient, n_k versus wavelength, λ for different hemoglobin concentrations. Both n_r and n_k increase with higher hemoglobin concentration across all wavelengths.	167
5.6	(a) Real part, ϵ_{rr} and (b) imaginary part, ϵ_{ri} of complex relative permittivity versus wavelength, λ : model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL. A good fit is observed between our proposed model and experimental data across all wavelengths.	170
5.7	(a) Real part, n_r and (b) imaginary part, n_i of complex refractive index versus wavelength, λ : model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL.	171
5.8	Absorption coefficient, μ_a versus wavelength, λ : model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL. .	172
5.9	Magnitude of (a) transmission and (b) reflection coefficients versus frequency for various CFLNs.	173
5.10	SAR (in logarithmic scale) at different locations of capillary at 440 THz (680 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.	176
5.11	SAR (in logarithmic scale) at different locations of capillary at 550 THz (545 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.	177
5.12	SAR (in logarithmic scale) at different locations of capillary at 720 THz (417 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.	178
5.13	(a) Real part of complex refractive index, n_r and (b) absorption coefficient, μ_a versus frequency for healthy skin and BCC. BCC generally has higher n_r and μ_a than healthy skin throughout the terahertz region.	180
5.14	Post-processed terahertz pulse from healthy skin and BCC computed using FADI-FDTD and explicit FDTD. The reflected terahertz pulse from BCC has a larger amplitude than the reflected terahertz pulse from healthy skin.	182

5.15	Illustration of the numerical scanning process and geometrical setup of human skin model.	183
5.16	Numerically scanned images of the normalized overall post-processed peak-to-peak terahertz pulse, E_{pp} for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area. Region with value of one indicates that of a healthy skin tissue.	186
5.17	Same as Fig. 5.16, but with roughness and irregularities on the surface of the human skin and edges of BCC patch.	187
5.18	Numerically scanned images of the normalized overall post-processed peak-to-peak terahertz pulse of elliptical BCC patch embedded within healthy skin with Debye parameters fitted to (a) maximum and (b) minimum experimental data.	188
5.19	Same as Fig. 5.18, but with added white Gaussian noise of SNR 32 dB to the reflected terahertz pulse.	189
5.20	Numerically scanned images of the normalized post-processed peak-to-peak terahertz pulse for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area. The filter function is chosen to only capture the frequency components of the reflected terahertz pulse from 0.35 to 0.55 THz.	190
5.21	Numerically scanned images of the normalized post-processed peak-to-peak terahertz pulse for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area. The BCC patches include the encrusted layer.	191
5.22	Numerically scanned images of the normalized overall post-processed peak-to-peak terahertz pulse of buried tumour, E_{btp} with the shape of (a) sphere and (b) 45 degree counter-clockwise rotated ellipsoid. Region with value of zero indicates that of a healthy skin tissue. . . .	193
5.23	Real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity for metal Au (gold): Drude model and experimental data.	195
5.24	Real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity for metal Au (gold): Drude-Lorentz model and experimental data. . .	196
5.25	Real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity for metal Ag (silver): Drude-Lorentz model and experimental data. .	197
5.26	Magnitude of transmission coefficient of the optical waveguide from photon energy 1.24 eV to 2.48 eV for various CFLNs.	199

5.27	Magnitude of transmission coefficient of the optical waveguide whereby its gold metal cladding is modeled separately as Drude-Lorentz and Drude model.	201
5.28	Magnitude of transmission coefficients of the optical waveguide with Au-air-Au and Ag-air-Ag interfaces.	202
5.29	Magnitude of transmission coefficients of the optical waveguide with Au-air-Au and Au-SiO ₂ -Au interfaces.	203
5.30	Configurations of conventional plasmonic waveguide grating filter. ©2010 IEEE.	203
5.31	Magnitude of transmission coefficient of conventional plasmonic waveguide grating filter from photon energy 0.52 eV to 1.1 eV.	204
5.32	Configurations of apodized plasmonic waveguide grating filter. ©2010 IEEE.	204
5.33	Magnitude of transmission coefficient of apodized plasmonic waveguide grating filter from photon energy 0.52 eV to 1.1 eV.	205
5.34	Configurations of chirped plasmonic waveguide grating filter. ©2010 IEEE.	205
5.35	Magnitude of transmission coefficient of chirped plasmonic waveguide grating filter from photon energy 0.52 eV to 1.1 eV.	206
5.36	Configurations of conventional plasmonic microcavity. ©2010 IEEE.	207
5.37	Configurations of apodized plasmonic microcavity. ©2010 IEEE.	207
5.38	Magnitude of transmission coefficient of apodized plasmonic microcavity from photon energy 0.52 eV to 1.1 eV.	208

List of Tables

3.1	Past literatures on stability analysis for Yee's explicit FDTD method.	43
3.2	Stability criterion and update coefficients for 3-D FDTD schemes. ©2010 IEEE.	50
3.3	CPU time incurred by different FDTD schemes. ©2010 IEEE.	54
3.4	Complex numerical permittivity and leading error term for FDTD schemes	56
3.5	Conversion among time, frequency and Z domains. ©2009 IEEE.	71
3.6	Memory storage requirements for Debye media. ©2009 IEEE.	78
3.7	Memory storage requirements for Lorentz media	83
3.8	List of complex numerical permittivity and leading error term for Debye media. ©2009 IEEE.	85
3.9	List of complex numerical permittivity and leading error term for Lorentz media	86
4.1	Matrices for various ADI-FDTD schemes for lossy media	117
4.2	Coefficients and parameters of update equations for various efficient FADI-FDTD schemes	122
4.3	Comparisons of number of arithmetic operations per grid between conventional and efficient fundametal forms of ADI-FDTD schemes for lossy media over one complete time step	123
4.4	Relative CPU time for various ADI-FDTD schemes for lossy media	129
4.5	Efficiency gain in terms of CPU time achieved by efficient fundamen- tal form over conventional form of ADI-FDTD and explicit FDTD for different computational domain sizes	129
4.6	Efficiency gain and relative root-mean-square error of efficient FADI- FDTD schemes for various CFLNs	134

4.7	Relative permittivity, ϵ_r and conductivity, σ of skin layers at 42.25 GHz and 61.22 GHz	135
5.1	Fitted values of a_p , r_p and ϵ_∞ for hemoglobin concentration of 15 g/dL	169
5.2	Fitted values of a_p , r_p and ϵ_∞ for hemoglobin concentration of 33 g/dL	169
5.3	Maximum and Average SAR values computed using FADI-FDTD and explicit FDTD at hemoglobin concentration of 15 g/dL	177
5.4	Maximum and Average SAR values computed using FADI-FDTD and explicit FDTD at hemoglobin concentration of 33 g/dL	178
5.5	Debye parameters for healthy skin and BCC in terahertz region . . .	180
5.6	Variation of Debye parameters for healthy skin fitted to maximum and minimum experimental data	187
5.7	Efficiency gain and relative root-mean-square (RMS) error of FADI-FDTD for various CFLNs	191
5.8	Parameters of Drude and Drude-Lorentz models for metal Au (gold) .	198
5.9	Parameters of Drude-Lorentz model for metal Ag (silver)	198
5.10	Efficiency gain and relative error of FADI-FDTD method for various CFLNs	199
5.11	Relative error of efficient FADI-FDTD schemes for various CFLNs and CPWs	200
6.1	Comparison among Yee's explicit FDTD, ADI-FDTD and FADI-FDTD methods	212

Chapter 1

Introduction

1.1 Motivation

The finite-difference time-domain (FDTD) method [1, 2] has gained much significance since the birth of cheap digital computer era, where computing powers and memory capacities have increased tremendously over the years. The immediate impacts are the prominent social requirements and future prospects of FDTD method. To describe some of them, FDTD finds a lot of applications in topics related to microwave photonics area. They include optical generation, distribution and control of microwave, millimeter-wave and terahertz (THz) signals, optically controlled microwave devices, monolithic integration of photonic and microwave electronic devices and circuits, components and channel analysis as well as optical/electrical interface and compatibility issues. In bioelectromagnetics, FDTD can be engaged in optical detection of early stage cancers and ultramicroscopy of individual living cells to investigate physiological processes. Application of noninvasive microwave imaging for detection of breast cancer at early stage can be modeled using FDTD. FDTD has also become a powerful tool for design of safe and efficient antennas for personal wireless communications devices, including cellphone to meet the safety standard requirement of human exposure to microwave radiation. Specific absorption rate

(SAR), which measures the electromagnetic energy absorption rate of human tissue exposed to electromagnetic radiation can be computed efficiently with the use of FDTD method. The ability of FDTD to model essentially arbitrary configurations of inhomogeneous, lossy and dispersive media results in its broad applicability in many engineering and science areas.

It is well known that the usage of such explicit FDTD method is limited by the fact that its time step is restricted by the Courant-Friedrich-Lewy (CFL) condition. If the spatial steps are small, this restriction may result in undesirably long simulation time. To overcome this problem, the alternating-direction-implicit FDTD (ADI-FDTD) method [3,4] was developed, which has unconditional stability feature. This method has attracted much interest because the time step is no longer restricted by the CFL condition and hence simulation time can be accelerated. Nevertheless, there still exists some persistent issues to be resolved. The stability analysis of explicit and implicit FDTD methods is performed mostly for only electrically lossy media. It appears that the full 3-D stability analysis of various possible FDTD schemes for the most general case of doubly lossy media, where both electric and magnetic conductivities coexist, are still lacking. The dispersion analysis is also mostly confined to electrically lossy media. On top of that, it is believed that there is still room for improvement on the accuracy of some existing FDTD schemes for lossy and dispersive media.

The introduction of ADI-FDTD method, which has unconditional stability feature is an important step toward improving the efficiency of FDTD methods. Unfortunately, due to the fact that the algorithm is implicit in nature, its implementation is rather complicated. Not only are there tridiagonal systems that need to be solved, the right-hand-side (RHS) of each equation involves many update coefficients and field variables, which calls for considerable arithmetic operations and memory in-

dexing. For lossy and dispersive media, the efficiency of the ADI-FDTD method is further reduced due to additional field variables and update coefficients. It is therefore hopeful that such efficiency degradation can be well addressed.

1.2 Objectives

Based on the motivation outlined in the preceding section. The objectives of the thesis are as follows:

- 1) To perform a thorough and generalized stability and dispersion analysis of FDTD methods of all schemes for doubly lossy media.
- 2) To improve on the accuracy of FDTD methods for lossy and dispersive media.
- 3) To improve on the efficiency of ADI-FDTD method for lossy and dispersive media.
- 4) Once the stability, accuracy and efficiency issues are well addressed, to demonstrate the applicability of the improved FDTD methods for lossy and dispersive media in many interesting engineering and science areas such as electromagnetic compatibility, bioelectromagnetics and photonics.

In short, the overall objectives of the thesis are that while maintaining stability, the FDTD methods should be accurate, efficient and robust in dealing with lossy and dispersive media.

1.3 Major Contributions

The thesis achieves several major contributions in which many of them have been published in peer-reviewed international journals. The contributions are summarized as follows.

The generalized stability criterion of 3-D Yee's explicit FDTD method for doubly lossy media has been found for all schemes. The schemes are time-average (TA), time-forward (TF), time-backward (TB) and exponential time differencing (ETD). It is reducible to either electrically lossy, magnetically lossy or lossless media. The dispersion characteristics of various FDTD schemes in doubly lossy media have also been investigated by performing the 3-D dispersion analysis.

The Z transform theory and impulse invariance have been applied across discipline from digital signal processing to FDTD method. The current Z-transform method used in Yee's explicit FDTD for dispersive media has been found to be inaccurate. This is because the method is based on the classical impulse invariance method in Z-transform theory, which is incorrect and inaccurate when the impulse response is discontinuous at initial time $t = 0$. The correction has been shown to be necessary for dispersive media which exhibit discontinuity at $t = 0$ in the time domain susceptibility function. A corrected Z-transform table has been provided to facilitate the conversion from frequency to Z domain. With the aid of the table, various formulations of FDTD update equations for dispersive media can be carried out conveniently. The use of corrected impulse invariance method has led to accuracy improvement over classical impulse invariance method in FDTD.

Lyapunov and matrix norm stability analysis have been applied on all ADI-FDTD schemes for doubly lossy media. Among the schemes considered are averaging, forward-backward, backward-forward, forward-forward, exponential time differencing and backward-backward. For schemes which are unconditionally stable, the rigorous analytical proof of unconditional stability has been provided. For schemes which are not unconditionally stable, the condition to guarantee stability has been determined.

An unified efficient fundamental ADI-FDTD (FADI-FDTD) schemes for lossy media

has been formulated. They are formulated in the simplest, most concise, most efficient, and most fundamental form of ADI-FDTD. Such efficient fundamental schemes have substantially less RHS update coefficients and field variables compared to the conventional ADI-FDTD schemes. Thus, they feature higher efficiency with reduced memory indexing and arithmetic operations. The novel scheme based on the ETD is introduced for the first time in efficient fundamental form of ADI-FDTD method, which also achieves higher accuracy compared to other schemes. Further, the generalized formulation of FADI-FDTD method for dispersive media has been provided. It is efficient, robust and applicable to Debye, Lorentz, Drude and general complex conjugate pole-residue pair models.

The applications of FADI-FDTD method in the areas of electromagnetic compatibility, bioelectromagnetics and photonics have been demonstrated. In electromagnetic compatibility, the modeling of reverberation chamber in mode-stirred operation has been presented. A time variant complex relative permittivity has been introduced such that the boundary conditions inside the chamber can be altered continuously, i.e., the mode-stirred operation. For application in bioelectromagnetics, the interaction of light with hemoglobin at optical frequency has been presented. An accurate model based on complex conjugate pole-residue pair has been proposed to model the complex permittivity of hemoglobin at optical frequency. The interaction of terahertz pulse with healthy skin and basal cell carcinoma (BCC) has also been demonstrated, where the human skin is modeled as Debye media. For application in photonics, the characteristics of a surface plasmon waveguides with Au (gold) and Ag (silver) metal cladding, modeled as combination of Drude-Lorentz dispersive media have been analyzed. Further analysis of plasmonic waveguide grating filter has also been considered. To sum up the contributions, the thesis has successfully developed a comprehensive FDTD-based computational framework which serves as a modeling and analysis platform for lossy and dispersive electromagnetic

problems.

1.4 Organization of the Thesis

The rest of the thesis is organized as follows.

Chapter 2 gives an overview of literature survey done on various areas related to the FDTD methods. The Maxwell's equations, which form the basis of electromagnetic theory is first introduced. The conventional Yee's explicit FDTD method as well as unconditionally stable ADI-FDTD method are reviewed and described. The incorporation of these FDTD methods in modeling electromagnetic wave propagation in lossy and dispersive media are included. The fundamentals of performing stability and dispersion analysis are detailed to facilitate the performance investigation of FDTD method.

Chapter 3 presents various aspects of Yee's explicit FDTD method for lossy and dispersive media. Firstly, the stability and dispersion analysis of 3-D Yee's explicit FDTD schemes for doubly lossy media is shown. A generalized stability criterion applicable for all 3-D Yee's explicit FDTD schemes is found. Furthermore, it is reducible to the case of either electrically lossy, magnetically lossy or even lossless media. The 3-D dispersion characteristics such as phase velocity and attenuation errors of various Yee's explicit FDTD schemes are also discussed. This is followed by thorough discussions of corrected impulse invariance method in the realm of Z transform theory for dispersive media. A Z-transform table is provided to supplement and *correct* the classical Z-transform tables. With the aid of the table, various formulations of FDTD update equations for dispersive media are carried out conveniently. Detailed performance measures such as numerical permittivity, leading error term, dispersion relation, normalized phase and attenuation errors as well as memory storage requirements are included along with some extensive numerical

comparisons.

Chapter 4 presents various aspects of fundamental ADI-FDTD (FADI-FDTD) method for lossy and dispersive media. Firstly, the Lyapunov and matrix norm stability analysis is applied to various ADI-FDTD schemes for doubly lossy media. The stability analysis is performed rigorously in both time and frequency domains. Among the schemes considered are averaging, forward-backward, backward-forward, forward-forward, exponential time differencing and backward-backward. Subsequently, the formulation of an unified efficient FADI-FDTD method for lossy media is detailed. Unifications of these schemes in both conventional and efficient fundamental forms of source-incorporated ADI-FDTD are provided. Other aspects such as field and parameter memory arrays, perfect electric conductor (PEC) and perfect magnetic conductor (PMC) implementations are also discussed. Numerical results which include CPU time saving (efficiency gain) as well as asymmetry and numerical errors are presented and discussed. The SAR computation of human skin exposed to electromagnetic radiation is also shown. Further, the generalized formulation of FADI-FDTD method for dispersive media is provided. Such generalized formulation is efficient, robust and is applicable to Debye, Lorentz, Drude and complex conjugate pole-residue pair models.

Chapter 5 demonstrates the applications of FADI-FDTD method in the areas of electromagnetic compatibility, bioelectromagnetics and photonics. In electromagnetic compatibility, the modeling of reverberation chamber in mode-stirred operation is presented. A time variant complex relative permittivity is introduced such that the boundary conditions inside the chamber can be altered continuously for mode-stirred operation. For application in bioelectromagnetics, the interaction of light with hemoglobin at optical frequency is presented. An accurate model based on complex conjugate pole-residue pair is proposed to model the complex permittiv-

ity of hemoglobin at optical frequency. Besides that, the interaction of terahertz pulse with healthy skin and basal cell carcinoma (BCC) is demonstrated, where the human skin is modeled as Debye media. For application in photonics, the characteristics of a surface plasmon waveguides with Au (gold) and Ag (silver) metal cladding, modeled as combination of Drude-Lorentz dispersive media is analyzed. Further analysis of plasmonic waveguide grating filter is also shown.

Finally, Chapter 6 provides the overall conclusions of the thesis and outlines some suggestions for future work.

Chapter 2

A Brief Literature Survey on FDTD Methods

This chapter gives an overview of literature survey done on various areas related to the FDTD methods. The Maxwell's equations, which form the basis of electromagnetic theory is first introduced. The conventional Yee's explicit FDTD method as well as unconditionally stable ADI-FDTD method are reviewed and described. The incorporation of these FDTD methods in modeling electromagnetic wave propagation in lossy media and linear dispersive media are included. The fundamentals of performing stability and dispersion analysis are detailed to facilitate the performance investigation of FDTD methods.

2.1 Maxwell's Equations

The time-dependent Maxwell's equations in differential and integral forms are given by

Differential form:

$$\nabla \cdot \mathbf{D} = \rho \quad (2.1.1a)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (2.1.1b)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} - \mathbf{M} \quad (2.1.1c)$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \quad (2.1.1d)$$

Integral form:

$$\oiint_S \mathbf{D} \cdot d\mathbf{S} = \iiint_V \rho dV = Q \quad (2.1.2a)$$

$$\oiint_S \mathbf{B} \cdot d\mathbf{S} = 0 \quad (2.1.2b)$$

$$\oint_L \mathbf{E} \cdot d\mathbf{L} = -\frac{\partial}{\partial t} \iint_S \mathbf{B} \cdot d\mathbf{S} - \iint_S \mathbf{M} \cdot d\mathbf{S} \quad (2.1.2c)$$

$$\oint_L \mathbf{H} \cdot d\mathbf{L} = \frac{\partial}{\partial t} \iint_S \mathbf{D} \cdot d\mathbf{S} + \iint_S \mathbf{J} \cdot d\mathbf{S} \quad (2.1.2d)$$

with the following symbols definition and units:

E: electric field vector (V/m)

D: electric flux density vector (C/m²)

H: magnetic field vector (A/m)

B: magnetic flux density vector (Wb/m²)

J: electric current density vector (A/m²)

M: equivalent magnetic current density (V/m²)

ρ : electric charge density (C/m³)

V : arbitrary volume in three-dimensional space

dV : differential volume

Q : total electric charge enclosed in V

S : arbitrary three-dimensional surface

$d\mathbf{S}$: differential normal vector for surface S (m^2)

L : closed contour of surface S

$d\mathbf{L}$: differential length vector for contour L (m)

In linear isotropic and nondispersive media, the following constitutive relations hold between the electric and magnetic fields and flux densities:

$$\mathbf{D} = \epsilon \mathbf{E} = \epsilon_0 \epsilon_r \mathbf{E} \quad (2.1.3a)$$

$$\mathbf{B} = \mu \mathbf{H} = \mu_0 \mu_r \mathbf{H} \quad (2.1.3b)$$

with the following parameters definition and units:

ϵ : electric permittivity (F/m)

ϵ_0 : free space permittivity ($8.854 \times 10^{-12} \text{ F/m}$)

ϵ_r : dimensionless relative permittivity

μ : magnetic permeability (H/m)

μ_0 : free space permeability ($4\pi \times 10^{-7} \text{ H/m}$)

μ_r : dimensionless relative permeability

Assuming $e^{j\omega t}$ time dependance where $j = \sqrt{-1}$, $\omega = 2\pi f$ and f represents frequency, the Maxwell's equations of differential form are oftenly expressed in phasor (Fourier) form as

$$\nabla \cdot \tilde{\mathbf{D}} = \rho \quad (2.1.4a)$$

$$\nabla \cdot \tilde{\mathbf{B}} = 0 \quad (2.1.4b)$$

$$\nabla \times \tilde{\mathbf{E}} = -j\omega \tilde{\mathbf{B}} - \tilde{\mathbf{M}} \quad (2.1.4c)$$

$$\nabla \times \tilde{\mathbf{H}} = j\omega \tilde{\mathbf{D}} + \tilde{\mathbf{J}} \quad (2.1.4d)$$

where the tilde sign indicates complex vectors. The Fourier transform and inverse Fourier transform can be used to convert the solution of Maxwell's equations from time domain to frequency domain and vice versa.

2.1.1 Lossy Media

For simplicity, assume a source-free region where $\rho = 0$, $\mathbf{J} = 0$ and $\mathbf{M} = 0$. In lossy media, although under the absence of independent current sources, there still exists electric conduction current density and its equivalent magnetic conduction current density

$$\mathbf{J} = \sigma \mathbf{E}; \quad \mathbf{M} = \sigma^* \mathbf{H} \quad (2.1.5)$$

where σ is the electric conductivity in S/m and σ^* is the equivalent magnetic conductivity in Ω/m . Substituting (2.1.5) into (2.1.1), the differential form of Maxwell's equations read:

$$\nabla \cdot \mathbf{D} = 0 \quad (2.1.6a)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (2.1.6b)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} - \sigma^* \mathbf{H} \quad (2.1.6c)$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \sigma \mathbf{E} \quad (2.1.6d)$$

In phasor form, the Maxwell's curl equations in (2.1.6c)-(2.1.6d) are commonly expressed as

$$\begin{aligned} \nabla \times \tilde{\mathbf{H}} &= j\omega\epsilon\tilde{\mathbf{E}} + \sigma\tilde{\mathbf{E}} \\ &= j\omega\epsilon_0 \left(\epsilon_r - j\frac{\sigma}{\epsilon_0\omega} \right) \tilde{\mathbf{E}} \end{aligned} \quad (2.1.7)$$

and

$$\begin{aligned} -\nabla \times \tilde{\mathbf{E}} &= j\omega\mu\tilde{\mathbf{H}} + \sigma^*\tilde{\mathbf{H}} \\ &= j\omega\mu_0 \left(\mu_r - j\frac{\sigma^*}{\mu_0\omega} \right) \tilde{\mathbf{H}} \end{aligned} \quad (2.1.8)$$

where the complex relative permittivity and permeability are introduced as

$$\epsilon_r(\omega) = \left(\epsilon_r - j\frac{\sigma}{\epsilon_0\omega} \right); \quad \mu_r(\omega) = \left(\mu_r - j\frac{\sigma^*}{\mu_0\omega} \right). \quad (2.1.9)$$

We shall focus on the differential form of Maxwell's curl equations (2.1.6c)-(2.1.6d) in three-dimensional Cartesian coordinate due to its relevance to the FDTD methods. To that end, (2.1.6c)-(2.1.6d) can be expanded into six coupled partial differential equations:

$$\frac{\partial E_x}{\partial t} = \frac{1}{\epsilon} \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x \right) \quad (2.1.10a)$$

$$\frac{\partial E_y}{\partial t} = \frac{1}{\epsilon} \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y \right) \quad (2.1.10b)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right) \quad (2.1.10c)$$

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \sigma^* H_x \right) \quad (2.1.10d)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - \sigma^* H_y \right) \quad (2.1.10e)$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \sigma^* H_z \right) \quad (2.1.10f)$$

The system of six coupled partial differential equations (2.1.10a)-(2.1.10f) form the basis of the FDTD methods in solving various electromagnetics problems in three-dimensional space.

2.1.2 Dispersive Media

In linear isotropic dispersive media, the simple constitutive relations in (2.1.3) no longer hold. Instead, the relations between electric and magnetic fields and flux densities are expressed in the frequency domain as

$$\tilde{\mathbf{D}} = \epsilon_0 \epsilon_r(\omega) \tilde{\mathbf{E}} \quad (2.1.11a)$$

$$\tilde{\mathbf{B}} = \epsilon_0 \mu_r(\omega) \tilde{\mathbf{H}} \quad (2.1.11b)$$

There are three notable types of dispersive media frequently used in the FDTD modeling at macroscopic scale, namely, Debye, Lorentz and Drude media. For simplicity, we assume only electrically dispersive media. The complex relative permittivities of these three different types of dispersive media are described as follows:

Debye

The complex relative permittivity, $\epsilon_r(\omega)$ of a Debye medium with multiple poles is characterized by

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p}{1 + j\omega\tau_p} \quad (2.1.12)$$

where ϵ_∞ is the relative permittivity at infinite frequency, $\Delta\epsilon_p$ is the change in relative permittivity due to the p -th Debye pole and τ_p is the p -th pole relaxation time. The time domain susceptibility function $\chi(t)$ is given as a decaying exponential function

$$\chi_p(t) = \frac{\Delta\epsilon_p}{\tau_p} e^{-t/\tau_p} u(t) \quad (2.1.13)$$

where $u(t)$ is the unit step function.

Lorentz

The frequency domain susceptibility function of a Lorentz medium has one or more pairs of complex-conjugate poles. The complex relative permittivity, $\epsilon_r(\omega)$ of a Lorentz medium with multiple complex conjugate pole pairs is characterized by

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p \omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2} \quad (2.1.14)$$

where $\Delta\epsilon_p$ is the change in relative permittivity due to the p -th Lorentz pole pair, ω_p is the resonant frequency of the p -th pole pair and δ_p is the damping coefficient of the p -th pole pair. The time domain susceptibility function $\chi(t)$ is obtained as an exponentially decaying sinusoidal function

$$\chi_p(t) = \frac{\Delta\epsilon_p \omega_p^2}{\sqrt{\omega_p^2 - \delta_p^2}} e^{-\delta_p t} \sin(\sqrt{\omega_p^2 - \delta_p^2} t) u(t). \quad (2.1.15)$$

Drude

Drude model is normally used to properly account for the physics of internal electron motion at optical wavelength. For a Drude medium with multiple poles, the complex relative permittivity, $\epsilon_r(\omega)$ is characterized by

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{-\omega_p^2}{\omega^2 - j\omega\nu_p} \quad (2.1.16)$$

where ω_p is the p -th Drude pole resonant frequency and ν_p is the p -th pole inverse relaxation time. The time domain susceptibility function $\chi(t)$ is obtained as

$$\chi_p(t) = \frac{\omega_p^2}{\nu_p} (1 - e^{-\nu_p t}) u(t) \quad (2.1.17)$$

Note that the FDTD update equations for dispersive media require special treatment and will be further discussed in Section 2.2.2.

2.2 Yee's Explicit FDTD Method

The Yee's explicit FDTD method was introduced by Kane Yee in 1966 [1], which uses a set of finite-difference equations to discretize the Maxwell's curl equations for lossless media, i.e. $\sigma = 0$ and $\sigma^* = 0$. In Yee's explicit FDTD method, the electric and magnetic fields are staggered in Yee's cell. The space time notation widely adopted is indicated as

$$u|_{i,j,k}^n = u(i\Delta x, j\Delta y, k\Delta z, n\Delta t) \quad (2.2.1)$$

where Δx , Δy and Δz are the spatial steps in x , y and z direction respectively, Δt is the time step. i , j , k and n are the associated spatial and time indices. In the following, we shall consider the Yee's explicit FDTD method for lossy media as well as its extensions to dispersive media.

2.2.1 For Lossy Media

Applying the finite-difference discretization to the Maxwell's curl equations in (2.1.10) for both time and space, taking into account the staggered electric and magnetic fields in Yee's cell, we arrive at the update equations of Yee's explicit FDTD method for lossy media.

$$\begin{aligned} E_x|_{i+\frac{1}{2},j,k}^{n+1} = & c_1 E_x|_{i+\frac{1}{2},j,k}^n \\ & + c_2 \left(\frac{H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - H_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta y} - \frac{H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i+\frac{1}{2},j,k-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z} \right) \end{aligned} \quad (2.2.2a)$$

$$\begin{aligned} E_y|_{i,j+\frac{1}{2},k}^{n+1} = & c_1 E_y|_{i,j+\frac{1}{2},k}^n \\ & + c_2 \left(\frac{H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z} - \frac{H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - H_z|_{i-\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta x} \right) \end{aligned} \quad (2.2.2b)$$

$$\begin{aligned}
E_z|_{i,j,k+\frac{1}{2}}^{n+1} &= c_1 E_z|_{i,j,k+\frac{1}{2}}^n \\
&+ c_2 \left(\frac{H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} - \frac{H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y} \right)
\end{aligned} \tag{2.2.2c}$$

$$\begin{aligned}
H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{3}{2}} &= d_1 H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} \\
&+ d_2 \left(\frac{E_y|_{i,j+\frac{1}{2},k+1}^{n+1} - E_y|_{i,j+\frac{1}{2},k}^{n+1}}{\Delta z} - \frac{E_z|_{i,j+1,k+\frac{1}{2}}^{n+1} - E_z|_{i,j,k+\frac{1}{2}}^{n+1}}{\Delta y} \right)
\end{aligned} \tag{2.2.2d}$$

$$\begin{aligned}
H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{3}{2}} &= d_1 H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} \\
&+ d_2 \left(\frac{E_z|_{i+1,j,k+\frac{1}{2}}^{n+1} - E_z|_{i,j,k+\frac{1}{2}}^{n+1}}{\Delta x} - \frac{E_x|_{i+\frac{1}{2},j,k+1}^{n+1} - E_x|_{i+\frac{1}{2},j,k}^{n+1}}{\Delta z} \right)
\end{aligned} \tag{2.2.2e}$$

$$\begin{aligned}
H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{3}{2}} &= d_1 H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} \\
&+ d_2 \left(\frac{E_x|_{i+\frac{1}{2},j+1,k}^{n+1} - E_x|_{i+\frac{1}{2},j,k}^{n+1}}{\Delta y} - \frac{E_y|_{i+1,j+\frac{1}{2},k}^{n+1} - E_y|_{i,j+\frac{1}{2},k}^{n+1}}{\Delta x} \right)
\end{aligned} \tag{2.2.2f}$$

where

$$c_1 = \frac{1 - \frac{\sigma \Delta t}{2\epsilon}}{1 + \frac{\sigma \Delta t}{2\epsilon}}; \quad c_2 = \frac{\frac{\Delta t}{\epsilon}}{1 + \frac{\sigma \Delta t}{2\epsilon}}; \tag{2.2.3a}$$

$$d_1 = \frac{1 - \frac{\sigma^* \Delta t}{2\mu}}{1 + \frac{\sigma^* \Delta t}{2\mu}}; \quad d_2 = \frac{\frac{\Delta t}{\mu}}{1 + \frac{\sigma^* \Delta t}{2\mu}}. \tag{2.2.3b}$$

We can see that any electric or magnetic fields components at the present time step can be calculated from the field components at the previous time steps, which makes the Yee's FDTD an explicit algorithm. Due to its explicit nature, the Yee's explicit FDTD is subjected to the CFL condition, which imposes a maximum constraint on its time step size. The CFL condition will be described in more detail in Section 2.4, which focuses on stability and dispersion analysis. In the above, the electric and magnetic fields associated with the electric and magnetic conductivities respectively are averaged between time indices of n and $n + 1$, which is commonly known as the time-averaging scheme [2]. Nonetheless, there exist other different schemes of choosing the time indices for electric and magnetic fields associated with the elec-

tric and magnetic conductivities, such as time-forward [5], time-backward [6] and exponential time differencing [7, 8]. These schemes shall be further elaborated in Chapter 3.

On top of that, there are many ways to generate electromagnetic wave sources for the use in Yee's explicit FDTD method. Hard sources can be set up by assigning a desired time function to specific components of $\mathbf{E}$ or $\mathbf{H}$. The convenient way is the direct use of electric current density, $\mathbf{J}$ and magnetic current density, $\mathbf{M}$ sources. For $\mathbf{J}$ and $\mathbf{M}$ sources, in addition to radiating fields, the FDTD grid can deposit charge and generate charge associated fields [9]. Plane wave source condition can also be realized in Yee's explicit FDTD by means of total-field/scattered-field (TF/SF) formulation [10–12]. Other sources such as the waveguide source condition can also be generated for the analysis of waveguides structure using FDTD method. The perfectly matched layer (PML), first introduced by Berenger in 1994 [13] is commonly used to terminate the computational boundaries of the Yee's explicit FDTD method. Other literatures on subsequent developments of the PML can also be found in [14–24].

2.2.2 Extensions to Dispersive Media

Generally, the dispersive characteristics of a material are given in terms of dispersive permittivity models, and some methods had been previously developed to incorporate the frequency dependent properties into the FDTD update equations [25–44]. The following subsections will give a general overview of some of the popular methods. These methods are generally categorized into three groups: recursive convolution (RC) based method [25–30], auxiliary differential equation (ADE) method [31–36] and Z-transform method [37–42]. Reference [45] presented a summary and systematic analysis of these methods for dispersive media. Reference [46]

further provided a review of time domain methods for solving electromagnetic problems in dispersive and complex media. For convenience, the subscript indices of all fields will be omitted in this section.

Piecewise Linear Recursive Convolution (PLRC) Method

Reference [27] reported the development of an approach to model electromagnetic wave propagation in dispersive media, whereby the convolution integral relating the D and E fields are discretized using a recursive accumulator. It is actually the improvement to its original work in [25] and [26]. The discretized E field is set as a piecewise linear function instead of mere constant value as in [25] and [26]. The accuracy is improved with essentially the same computational complexity. The algorithm works as follows.

The convolution between the discrete time form of electric flux density and electric field intensity is written as

$$\mathbf{D}^n = \epsilon_0 \epsilon_\infty \mathbf{E}^n + \epsilon_0 \int_{\tau=0}^{n\Delta t} \mathbf{E}(n\Delta t - \tau) \chi(\tau) d\tau \quad (2.2.4)$$

At any given time interval between $i\Delta t$ and $(i+1)\Delta t$, $\mathbf{E}(t)$ can be approximated by linearly interpolating the values of $\mathbf{E}$ at the beginning and end of the time interval as

$$\mathbf{E}(t) = \mathbf{E}^i + \left(\frac{\mathbf{E}^{i+1} - \mathbf{E}^i}{\Delta t} \right) \cdot (t - i\Delta t). \quad (2.2.5)$$

Rewriting (2.2.5) in a time-reversed and offset form such that it conforms to the form of E in the convolution integral of (2.2.4), we get

$$\mathbf{E}(n\Delta t - \tau) = \mathbf{E}^{n-m} + \left(\frac{\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}}{\Delta t} \right) \cdot (\tau - m\Delta t). \quad (2.2.6)$$

Substituting (2.2.6) into (2.2.4), we obtain after some manipulations

$$\mathbf{D}^n = \epsilon_0 \epsilon_\infty \mathbf{E}^n + \epsilon_0 \sum_{m=0}^{n-1} \left[\mathbf{E}^{n-m} \chi^m + (\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}) \xi^m \right] \quad (2.2.7)$$

where

$$\chi^m = \int_{m\Delta t}^{(m+1)\Delta t} \chi(\tau) d\tau; \quad \xi^m = \frac{1}{\Delta t} \int_{m\Delta t}^{(m+1)\Delta t} (\tau - m\Delta t) \chi(\tau) d\tau \quad (2.2.8)$$

Subsequently, the expressions of $\mathbf{D}^n$ and $\mathbf{D}^{n+1}$ in (2.2.7) are substituted into the discrete time Ampere's law

$$\nabla \times \mathbf{H}^{n+\frac{1}{2}} = \frac{\mathbf{D}^{n+1} - \mathbf{D}^n}{\Delta t} \quad (2.2.9)$$

and we arrive at the general form of FDTD update equation for E field:

$$\begin{aligned} \mathbf{E}^{n+1} = & \left(\frac{\epsilon_\infty - \xi^0}{\epsilon_\infty - \xi^0 + \chi^0} \right) \mathbf{E}^n + \left(\frac{\Delta t / \epsilon_0}{\epsilon_\infty - \xi^0 + \chi^0} \right) \nabla \times \mathbf{H}^{n+\frac{1}{2}} \\ & + \left(\frac{1}{\epsilon_\infty - \xi^0 + \chi^0} \right) \sum_{m=0}^{n-1} \left[\mathbf{E}^{n-m} \Delta \chi^m + (\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}) \Delta \xi^m \right] \end{aligned} \quad (2.2.10)$$

where

$$\Delta \chi^m = \chi^m - \chi^{m+1}; \quad \Delta \xi^m = \xi^m - \xi^{m+1} \quad (2.2.11)$$

We now designate the summation in (2.2.10) as a new vector variable ψ :

$$\psi^n = \sum_{m=0}^{n-1} \left[\mathbf{E}^{n-m} \Delta \chi^m + (\mathbf{E}^{n-m-1} - \mathbf{E}^{n-m}) \Delta \xi^m \right] \quad (2.2.12)$$

This can be efficiently evaluated using a recursion relation of the form

$$\psi_p^n = (\Delta \chi_p^0 - \Delta \xi_p^0) \mathbf{E}^n + \Delta \xi_p^0 \mathbf{E}^{n-1} + C_p^{rec} \psi_p^{n-1} \quad (2.2.13)$$

where χ_p^0 , $\Delta \xi_p^0$ and C_p^{rec} are real-valued constants for Debye media and complex-valued for Lorentz media as will be shown later. The final E field update equation

now reads:

$$\begin{aligned} \mathbf{E}^{n+1} = & \left(\frac{\epsilon_\infty - \sum_p \xi^0 - \frac{\sigma \Delta t}{2\epsilon_0}}{\epsilon_\infty - \sum_p \xi^0 + \sum_p \chi^0 + \frac{\sigma \Delta t}{2\epsilon_0}} \right) \mathbf{E}^n \\ & + \left(\frac{\Delta t / \epsilon_0}{\epsilon_\infty - \sum_p \xi^0 + \sum_p \chi^0 + \frac{\sigma \Delta t}{2\epsilon_0}} \right) \nabla \times \mathbf{H}^{n+\frac{1}{2}} \\ & + \left(\frac{1}{\epsilon_\infty - \sum_p \xi^0 + \sum_p \chi^0 + \frac{\sigma \Delta t}{2\epsilon_0}} \right) \sum_p \psi^n \end{aligned} \quad (2.2.14)$$

Formulation for Debye Media:

We now determine the expressions of χ^m , $\Delta\chi^m$, ξ^m , $\Delta\xi^m$ and C_p^{rec} for Debye media. These expressions depend on the susceptibility function of the dispersive medium. Substituting the time domain susceptibility function of Debye media in (2.1.13) into (2.2.8), we obtain for p -th Debye pole:

$$\chi_p^m = \Delta\epsilon_p \left(1 - e^{-\Delta t / \tau_p} \right) e^{-m\Delta t / \tau_p} \quad (2.2.15a)$$

$$\xi_p^m = \frac{\Delta\epsilon_p \tau_p}{\Delta t} \left[1 - (\Delta t / \tau_p + 1) e^{-\Delta t / \tau_p} \right] e^{-m\Delta t / \tau_p} \quad (2.2.15b)$$

The expressions for $\Delta\chi^m$ and $\Delta\xi^m$ can then be found using (2.2.8) in (2.2.11). The values of χ_p^0 , ξ_p^0 , $\Delta\chi^0$ and $\Delta\xi^0$ needed in the final E field update equation of (2.2.14) by setting $m = 0$.

To obtain C_p^{rec} , we follow the similar procedure outlined in appendix of [26] and obtain the recursion relation for ψ_p as

$$\psi_p^n = \left(\Delta\chi_p^0 - \Delta\xi_p^0 \right) \mathbf{E}^n + \Delta\xi_p^0 \mathbf{E}^{n-1} + \psi_p^{n-1} e^{-\Delta t / \tau_p} \quad (2.2.16)$$

which gives $C_p^{rec} = e^{-\Delta t / \tau_p}$.

Formulation for Lorentz Media:

For Lorentz media, a complex time domain susceptibility function is first introduced

as

$$\hat{\chi}_p(t) = -j\gamma_p e^{(-\alpha_p + j\beta_p)t} u(t) \quad (2.2.17)$$

where the carat sign here indicates complex value and

$$\alpha_p = \delta_p; \quad \beta_p = \sqrt{\omega_p^2 - \delta_p^2}; \quad \gamma_p = \Delta\epsilon_p \omega_p^2 / \beta_p \quad (2.2.18)$$

It is clear from (2.1.15) and (2.2.17) that $\chi_p(t) = \text{Re}(\hat{\chi}_p(t))$. Substituting $\hat{\chi}_p(t)$ for $\chi_p(t)$ in (2.2.8), we obtain for the p -th Lorentz pole pair

$$\hat{\chi}_p^m = \frac{-j\gamma_p}{\alpha_p - j\beta_p} \left[1 - e^{(-\alpha_p + j\beta_p)\Delta t} \right] e^{(-\alpha_p + j\beta_p)m\Delta t} \quad (2.2.19a)$$

$$\hat{\xi}_p^m = \frac{j\gamma_p/\Delta t}{(\alpha_p + \beta_p)^2} \left\{ [(\alpha_p - j\beta_p)\Delta t + 1] e^{(-\alpha_p + j\beta_p)\Delta t} - 1 \right\} e^{(-\alpha_p + j\beta_p)m\Delta t} \quad (2.2.19b)$$

and they are related to the real-valued counterparts χ_p^m and ξ_p^m by

$$\chi_p^m = \text{Re}(\hat{\chi}_p^m); \quad \xi_p^m = \text{Re}(\hat{\xi}_p^m). \quad (2.2.20)$$

The values of χ_p^0 and ξ_p^0 are then found by setting $m = 0$.

For Lorentz media, the recursive relation of (2.2.13) now becomes

$$\hat{\psi}_p^n = (\Delta\hat{\chi}_p^0 - \Delta\hat{\xi}_p^0) \mathbf{E}^n + \Delta\hat{\xi}_p^0 \mathbf{E}^{n-1} + \hat{\psi}_p^{n-1} e^{(-\alpha_p + j\beta_p)\Delta t} \quad (2.2.21)$$

with the following complex-valued definitions:

$$\Delta\hat{\chi}^m = \hat{\chi}^m - \hat{\chi}^{m+1}; \quad \Delta\hat{\xi}^m = \hat{\xi}^m - \hat{\xi}^{m+1} \quad (2.2.22)$$

Similarly, $\Delta\hat{\chi}^0$ and $\Delta\hat{\xi}^0$ are obtained by setting $m = 0$.

Finally, the real-valued ψ_p^n needed in the final E field update equation of (2.2.14) is obtained via

$$\psi_p^n = \text{Re}(\hat{\psi}_p^n). \quad (2.2.23)$$

Auxiliary Differential Equation (ADE) Method

The next method for implementing FDTD in dispersive media utilizes time domain auxiliary differential equations linking the polarization and the electric flux density [33, 34]. These equations are time stepped in synchronism with Maxwell's curl equations. Later on, [35] reported an efficient reformulation of ADE method with more simplicity and efficiency. The formulations of ADE method for Debye, Lorentz and Drude media are discussed as follows:

Formulation for Debye Media:

The Ampere's law of Maxwell's curl equation in time domain is first written down as

$$\begin{aligned}\nabla \times \mathbf{H}(t) &= \epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}(t)}{\partial t} + \sigma \mathbf{E}(t) + \sum_p \mathcal{F}^{-1} \left(\frac{j\omega \Delta \epsilon_p}{1 + j\omega \tau_p} \right) \\ &= \epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}(t)}{\partial t} + \sigma \mathbf{E}(t) + \sum_p \mathbf{J}_p(t)\end{aligned}\quad (2.2.24)$$

where $\mathcal{F}^{-1}$ represents inverse Fourier transform operation and $\mathbf{J}_p(t)$ is the introduced auxiliary variables associated with the p -th Debye pole. $\mathbf{J}_p(t)$ is related to $\mathbf{E}(t)$ by the following equation:

$$\mathbf{J}_p(t) + \tau_p \frac{\partial \mathbf{J}_p(t)}{\partial t} = \epsilon_0 \Delta \epsilon_p \frac{\partial \mathbf{E}(t)}{\partial t} \quad (2.2.25)$$

(2.2.25) is then discretized using the central difference approximation (at time index $n + \frac{1}{2}$) to yield

$$\mathbf{J}_p^{n+1} = k_{1p} \mathbf{J}_p^n + k_{2p} \left(\frac{\mathbf{E}^{n+1} - \mathbf{E}^n}{\Delta t} \right) \quad (2.2.26)$$

where

$$k_{1p} = \frac{1 - \Delta t/2\tau_p}{1 + \Delta t/2\tau_p}; \quad k_{2p} = \frac{\epsilon_0 \Delta \epsilon_p \Delta t / \tau_p}{1 + \Delta t/2\tau_p}. \quad (2.2.27)$$

To update (2.2.26) in synchronism with (2.2.24), we again make use of the semi-implicit approximation:

$$\mathbf{J}_p^{n+\frac{1}{2}} = \frac{1}{2} (\mathbf{J}_p^n + \mathbf{J}_p^{n+1}) = \frac{1}{2} \left[(1 + k_{1p}) \mathbf{J}_p^n + \frac{k_{2p}}{\Delta t} (\mathbf{E}^{n+1} - \mathbf{E}^n) \right]. \quad (2.2.28)$$

Combining (2.2.28) with the discretization of (2.2.24) and upon collecting like terms, we arrive at the final update equation for $\mathbf{E}$ field:

$$\mathbf{E}^{n+1} = c_1 \mathbf{E}^n + c_2 \left[\nabla \times \mathbf{H}^{n+\frac{1}{2}} - \frac{1}{2} \sum_p (1 + k_{1p}) \mathbf{J}_p^n \right] \quad (2.2.29)$$

where

$$c_1 = \frac{2\epsilon_0\epsilon_\infty + \sum_p k_{2p} - \sigma\Delta t}{2\epsilon_0\epsilon_\infty + \sum_p k_{2p} + \sigma\Delta t} \quad (2.2.30a)$$

$$c_2 = \frac{2\Delta t}{2\epsilon_0\epsilon_\infty + \sum_p k_{2p} + \sigma\Delta t}. \quad (2.2.30b)$$

Formulation for Lorentz Media:

The Ampere's law of Maxwell's curl equation in time domain is first written down as

$$\begin{aligned} \nabla \times \mathbf{H}(t) &= \epsilon_0\epsilon_\infty \frac{\partial \mathbf{E}(t)}{\partial t} + \sigma \mathbf{E}(t) + \sum_p \mathcal{F}^{-1} \left(\frac{j\omega\epsilon_0\Delta\epsilon_p\omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2} \right) \\ &= \epsilon_0\epsilon_\infty \frac{\partial \mathbf{E}(t)}{\partial t} + \sigma \mathbf{E}(t) + \sum_p \mathbf{J}_p(t) \end{aligned} \quad (2.2.31)$$

where $\mathbf{J}_p$ is now related to $\mathbf{E}$ by

$$\omega_p^2 \mathbf{J}_p(t) + 2\delta_p \frac{\partial \mathbf{J}_p(t)}{\partial t} + \frac{\partial^2 \mathbf{J}_p(t)}{\partial t^2} = \epsilon_0\Delta\epsilon_p\omega_p^2 \frac{\partial \mathbf{E}(t)}{\partial t} \quad (2.2.32)$$

(2.2.32) is then discretized using the central difference approximation (at time index $n + \frac{1}{2}$) to yield

$$\mathbf{J}_p^{n+1} = k_{1p} \mathbf{J}_p^n + k_{2p} \mathbf{J}_p^{n-1} + k_{3p} \left(\frac{\mathbf{E}^{n+1} - \mathbf{E}^{n-1}}{2\Delta t} \right) \quad (2.2.33)$$

where

$$k_{1p} = \frac{2 - \omega_p^2 \Delta t^2}{1 + \delta_p \Delta t}; \quad k_{2p} = \frac{\delta_p \Delta t - 1}{\delta_p \Delta t + 1}; \quad k_{3p} = \frac{\epsilon_0 \Delta \epsilon_p \omega_p^2 \Delta t^2}{1 + \delta_p \Delta t} \quad (2.2.34)$$

To update (2.2.33) in synchronism with (2.2.31), we again make use of the semi-implicit approximation:

$$\mathbf{J}_p^{n+\frac{1}{2}} = \frac{1}{2} (\mathbf{J}_p^n + \mathbf{J}_p^{n+1}) = \frac{1}{2} \left[(1 + k_{1p}) \mathbf{J}_p^n + k_{2p} \mathbf{J}_p^{n-1} + \frac{k_{3p}}{2\Delta t} (\mathbf{E}^{n+1} - \mathbf{E}^{n-1}) \right]. \quad (2.2.35)$$

Combining (2.2.35) with the discretization of (2.2.31) and upon collecting like terms, we arrive at the final update equation for $\mathbf{E}$ field:

$$\mathbf{E}^{n+1} = c_1 \mathbf{E}^{n-1} + c_2 \mathbf{E}^n + c_3 \left\{ \nabla \times \mathbf{H}^{n+\frac{1}{2}} - \frac{1}{2} \sum_p [(1 + k_{1p}) \mathbf{J}_p^n + k_{2p} \mathbf{J}_p^{n-1}] \right\} \quad (2.2.36)$$

where

$$c_1 = \frac{\frac{1}{2} \sum_p k_{3p}}{2\epsilon_0 \epsilon_\infty + \frac{1}{2} \sum_p k_{3p} + \sigma \Delta t} \quad (2.2.37a)$$

$$c_2 = \frac{2\epsilon_0 \epsilon_\infty - \sigma \Delta t}{2\epsilon_0 \epsilon_\infty + \frac{1}{2} \sum_p k_{3p} + \sigma \Delta t} \quad (2.2.37b)$$

$$c_3 = \frac{2\Delta t}{2\epsilon_0 \epsilon_\infty + \frac{1}{2} \sum_p k_{3p} + \sigma \Delta t} \quad (2.2.37c)$$

Note that for Lorentz media formulation, more field memory arrays is required due to the additional storage for $\mathbf{E}^{n-1}$ and $\mathbf{J}_p^{n-1}$.

Formulation for Drude Media:

The Ampere's law of Maxwell's curl equation in time domain is first written down as

$$\begin{aligned} \nabla \times \mathbf{H}(t) &= \epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}(t)}{\partial t} + \sigma \mathbf{E}(t) + \sum_p \mathcal{F}^{-1} \left(\frac{-j\omega \epsilon_0 \omega_p^2}{\omega^2 - j\omega \nu_p} \right) \\ &= \epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}(t)}{\partial t} + \sigma \mathbf{E}(t) + \sum_p \mathbf{J}_p(t) \end{aligned} \quad (2.2.38)$$

where $\mathbf{J}_p$ is now related to $\mathbf{E}$ by

$$\frac{\partial^2 \mathbf{J}_p(t)}{\partial t^2} + \nu_p \frac{\partial \mathbf{J}_p(t)}{\partial t} = \epsilon_0 \omega_p^2 \frac{\partial \mathbf{E}(t)}{\partial t} \quad (2.2.39)$$

Integrating once with respect to time and omitting the trivial constant solution, (2.2.39) is simplified into

$$\frac{\partial \mathbf{J}_p(t)}{\partial t} + \nu_p \mathbf{J}_p(t) = \epsilon_0 \omega_p^2 \mathbf{E}(t) \quad (2.2.40)$$

(2.2.40) is then discretized using the central difference approximation (at time index $n + \frac{1}{2}$) to yield

$$\mathbf{J}_p^{n+1} = k_{1p} \mathbf{J}_p^n + k_{2p} (\mathbf{E}^{n+1} + \mathbf{E}^n) \quad (2.2.41)$$

where

$$k_{1p} = \frac{1 - \nu_p \Delta t/2}{1 + \nu_p \Delta t/2}; \quad k_{2p} = \frac{\epsilon_0 \omega_p^2 \Delta t/2}{1 + \nu_p \Delta t/2} \quad (2.2.42)$$

To update (2.2.41) in synchronism with (2.2.38), we again make use of the semi-implicit approximation:

$$\mathbf{J}_p^{n+\frac{1}{2}} = \frac{1}{2} (\mathbf{J}_p^n + \mathbf{J}_p^{n+1}) = \frac{1}{2} \left[(1 + k_{1p}) \mathbf{J}_p^n + \frac{k_{2p}}{\Delta t} (\mathbf{E}^{n+1} - \mathbf{E}^n) \right]. \quad (2.2.43)$$

Combining (2.2.43) with the discretization of (2.2.38) and upon collecting like terms, we arrive at the final update equation for E field:

$$\mathbf{E}^{n+1} = c_1 \mathbf{E}^n + c_2 \left[\nabla \times \mathbf{H}^{n+\frac{1}{2}} - \frac{1}{2} \sum_p (1 + k_{1p}) \mathbf{J}_p^n \right] \quad (2.2.44)$$

where

$$c_1 = \frac{2\epsilon_0\epsilon_\infty - \Delta t \sum_p k_{2p} - \sigma \Delta t}{2\epsilon_0\epsilon_\infty + \Delta t \sum_p k_{2p} + \sigma \Delta t} \quad (2.2.45a)$$

$$c_2 = \frac{2\Delta t}{2\epsilon_0\epsilon_\infty + \Delta t \sum_p k_{2p} + \sigma \Delta t}. \quad (2.2.45b)$$

Z-Transform Method

The Z-transform method proposed in [37] and [38] is another viable approach which converts the transfer functions in the frequency domain into Z domain via a table of conversion and the update equations can be obtained conveniently. The formulation for Debye, Lorentz and Drude are detailed as follows:

Formulation for Debye Media:

The complex relative permittivity in frequency domain can be expressed as

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p}{1 + j\omega\tau_p} + \frac{\sigma}{j\omega\epsilon_0} \quad (2.2.46)$$

where we have also included the electric conductivity term.

With reference to the table provided in [37], the complex relative permittivity in frequency domain of (2.2.46) can be converted into Z domain as

$$\epsilon_r(z) = \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p\Delta t/\tau_p}{1 - e^{-\Delta t/\tau_p}z^{-1}} + \frac{\sigma\Delta t/\epsilon_0}{1 - z^{-1}} \quad (2.2.47)$$

Now, we write down the relationship between $\tilde{\mathbf{D}}(z)$ and $\tilde{\mathbf{E}}(z)$ in Z domain as

$$\begin{aligned} \tilde{\mathbf{D}}(z) &= \epsilon_0\epsilon_r(z)\tilde{\mathbf{E}}(z) \\ &= \epsilon_0 \left(\epsilon_\infty + \sum_p \frac{\Delta\epsilon_p\Delta t/\tau_p}{1 - e^{-\Delta t/\tau_p}z^{-1}} + \frac{\sigma\Delta t/\epsilon_0}{1 - z^{-1}} \right) \cdot \tilde{\mathbf{E}}(z) \end{aligned} \quad (2.2.48a)$$

Upon some expansion in the similar fashion as [37], we obtain

$$\begin{aligned} \tilde{\mathbf{D}}(z) &= \epsilon_0\epsilon_\infty\tilde{\mathbf{E}}(z) + \sum_p \frac{\epsilon_0\Delta\epsilon_p\Delta t}{\tau_p} \left(1 + \frac{e^{-\Delta t/\tau_p}z^{-1}}{1 - e^{-\Delta t/\tau_p}z^{-1}} \right) \tilde{\mathbf{E}}(z) \\ &\quad + \sigma\Delta t \left(1 + \frac{z^{-1}}{1 - z^{-1}} \right) \tilde{\mathbf{E}}(z). \end{aligned} \quad (2.2.49)$$

We also introduce two intermediate variables $\tilde{\mathbf{S}}_p(z)$ and $\tilde{\mathbf{I}}(z)$ with the following

definitions:

$$\tilde{\mathbf{S}}_p(z) = \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} \left(\frac{e^{-\Delta t/\tau_p}}{1 - e^{-\Delta t/\tau_p} z^{-1}} \right) \tilde{\mathbf{E}}(z) \quad (2.2.50a)$$

$$\tilde{\mathbf{I}}(z) = \left(\frac{\sigma \Delta t}{1 - z^{-1}} \right) \tilde{\mathbf{E}}(z) \quad (2.2.50b)$$

which help simplify (2.2.49) into

$$\tilde{\mathbf{D}}(z) = \epsilon_0 \epsilon_\infty \tilde{\mathbf{E}}(z) + \sum_p \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} \tilde{\mathbf{E}}(z) + \sigma \Delta t \tilde{\mathbf{E}}(z) + z^{-1} \sum_p \tilde{\mathbf{S}}_p(z) + z^{-1} \tilde{\mathbf{I}}(z) \quad (2.2.51)$$

Upon collecting the like terms, we arrive at the following set of Z domain equations:

$$\tilde{\mathbf{E}}(z) = \frac{\tilde{\mathbf{D}}(z) - z^{-1} \sum_p \tilde{\mathbf{S}}_p(z) - z^{-1} \tilde{\mathbf{I}}(z)}{\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} + \sigma \Delta t} \quad (2.2.52a)$$

$$\tilde{\mathbf{S}}_p(z) = e^{-\Delta t/\tau_p} z^{-1} \tilde{\mathbf{S}}_p(z) + \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} e^{-\Delta t/\tau_p} \tilde{\mathbf{E}}(z) \quad (2.2.52b)$$

$$\tilde{\mathbf{I}}(z) = z^{-1} \tilde{\mathbf{I}}(z) + \sigma \Delta t \tilde{\mathbf{E}}(z) \quad (2.2.52c)$$

The update equations in time domain can then be easily obtained from the above set of Z domain equations by recognizing that the z^{-1} operator denotes the value at one time step earlier. Combining (2.2.52) with the discretization of Ampere's law, the final update equation for E field read:

$$\mathbf{D}^{n+1} = \mathbf{D}^n + \nabla \times \mathbf{H}^{n+\frac{1}{2}} \quad (2.2.53a)$$

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} - \sum_p \mathbf{S}_p^n - \mathbf{I}^n}{\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} + \sigma \Delta t} \quad (2.2.53b)$$

$$\mathbf{S}_p^{n+1} = e^{-\Delta t/\tau_p} \mathbf{S}_p^n + \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} e^{-\Delta t/\tau_p} \mathbf{E}^{n+1}, \quad \forall p \quad (2.2.53c)$$

$$\mathbf{I}^{n+1} = \mathbf{I}^n + \sigma \Delta t \mathbf{E}^{n+1}. \quad (2.2.53d)$$

Formulation for Lorentz Media:

The complex relative permittivity in frequency domain can be expressed as

$$\begin{aligned}\epsilon_r(\omega) &= \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p \omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2} + \frac{\sigma}{j\omega\epsilon_0} \\ &= \epsilon_\infty + \sum_p \frac{\beta_p \gamma_p}{\alpha_p^2 + \beta_p^2 + 2j\omega\alpha_p - \omega^2} + \frac{\sigma}{j\omega\epsilon_0}\end{aligned}\quad (2.2.54)$$

where we have also included the electric conductivity term and

$$\alpha_p = \delta_p; \quad \beta_p = \sqrt{\omega_p^2 - \delta_p^2}; \quad \gamma_p = \Delta\epsilon_p \omega_p^2 / \beta_p \quad (2.2.55)$$

With reference to the table provided in [37], the complex relative permittivity in frequency domain of (2.2.54) can be converted into Z domain as

$$\epsilon_r(z) = \epsilon_\infty + \sum_p \frac{\Delta t \gamma_p e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t) z^{-1}}{1 - 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) z^{-1} + e^{-2\alpha_p \Delta t} z^{-2}} + \frac{\sigma \Delta t / \epsilon_0}{1 - z^{-1}} \quad (2.2.56)$$

Following the procedures in Debye media and upon collecting the like terms, we arrive at the following set of Z domain equations:

$$\tilde{\mathbf{E}}(z) = \frac{\tilde{\mathbf{D}}(z) - z^{-1} \sum_p \tilde{\mathbf{S}}_p(z) - z^{-1} \tilde{\mathbf{I}}(z)}{\epsilon_0 \epsilon_\infty + \sigma \Delta t} \quad (2.2.57a)$$

$$\begin{aligned}\tilde{\mathbf{S}}_p(z) &= 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) z^{-1} \tilde{\mathbf{S}}_p(z) - e^{-2\alpha_p \Delta t} z^{-2} \tilde{\mathbf{S}}_p(z) \\ &\quad + \Delta t \epsilon_0 \gamma_p e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t) \tilde{\mathbf{E}}(z)\end{aligned}\quad (2.2.57b)$$

$$\tilde{\mathbf{I}}(z) = z^{-1} \tilde{\mathbf{I}}(z) + \sigma \Delta t \tilde{\mathbf{E}}(z) \quad (2.2.57c)$$

The update equations in time domain can then be easily obtained from the above set of Z domain equations by recognizing that the z^{-1} and z^{-2} operators denote the value at one and two time steps earlier, respectively. Combining (2.2.57) with the discretization of Ampere's law, the final update equation for E field read:

$$\mathbf{D}^{n+1} = \mathbf{D}^n + \nabla \times \mathbf{H}^{n+\frac{1}{2}} \quad (2.2.58a)$$

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} - \sum_p \mathbf{S}_p^n - \mathbf{I}^n}{\epsilon_0 \epsilon_\infty + \sigma \Delta t} \quad (2.2.58b)$$

$$\mathbf{S}_p^{n+1} = 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) \mathbf{S}_p^n - e^{-2\alpha_p \Delta t} \mathbf{S}_p^{n-1} + \Delta t \epsilon_0 \gamma_p e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t) \mathbf{E}^{n+1}, \quad \forall p \quad (2.2.58c)$$

$$\mathbf{I}^{n+1} = \mathbf{I}^n + \sigma \Delta t \mathbf{E}^{n+1} \quad (2.2.58d)$$

Formulation for Drude Media:

The complex relative permittivity in frequency domain can be expressed as

$$\begin{aligned} \epsilon_r(\omega) &= \epsilon_\infty + \sum_p \frac{-\omega_p^2}{\omega^2 - j\omega\nu_p} + \frac{\sigma}{j\omega\epsilon_0} \\ &= \epsilon_\infty - \sum_p \frac{\omega_p^2/\nu_p}{\nu_p + j\omega} + \frac{\sum_p \omega_p^2/\nu_p + \sigma/\epsilon_0}{j\omega} \end{aligned} \quad (2.2.59)$$

where we have also included the electric conductivity term.

With reference to the table provided in [37], the complex relative permittivity in frequency domain of (2.2.59) can be converted into Z domain as

$$\epsilon_r(z) = \epsilon_\infty - \sum_p \frac{\Delta t \omega_p^2/\nu_p}{1 - e^{-\nu_p \Delta t} z^{-1}} + \frac{\sum_p \Delta t \omega_p^2/\nu_p + \sigma \Delta t/\epsilon_0}{1 - z^{-1}} \quad (2.2.60)$$

Following the procedures in Debye media and upon collecting the like terms, we arrive at the following set of Z domain equations:

$$\tilde{\mathbf{E}}(z) = \frac{\tilde{\mathbf{D}}(z) + z^{-1} \sum_p \tilde{\mathbf{S}}_p(z) - z^{-1} \tilde{\mathbf{I}}_p(z)}{\epsilon_0 \epsilon_\infty + \sigma \Delta t} \quad (2.2.61a)$$

$$\tilde{\mathbf{S}}_p(z) = e^{-\nu_p \Delta t} z^{-1} \tilde{\mathbf{S}}_p(z) + \frac{\epsilon_0 \Delta t \omega_p^2}{\nu_p} e^{-\nu_p \Delta t} \tilde{\mathbf{E}}(z) \quad (2.2.61b)$$

$$\tilde{\mathbf{I}}(z) = z^{-1} \tilde{\mathbf{I}}(z) + \left(\sum_p \frac{\epsilon_0 \Delta t \omega_p^2}{\nu_p} + \sigma \Delta t \right) \tilde{\mathbf{E}}(z) \quad (2.2.61c)$$

The update equations in time domain can then be easily obtained from the above set of Z domain equations by recognizing that the z^{-1} operator denotes the value at one time step earlier. Combining (2.2.61) with the discretization of Ampere's law, the final update equation for E field read:

$$\mathbf{D}^{n+1} = \mathbf{D}^n + \nabla \times \mathbf{H}^{n+\frac{1}{2}} \quad (2.2.62a)$$

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} + \sum_p \mathbf{S}_p^n - \mathbf{I}_p^n}{\epsilon_0 \epsilon_\infty + \sigma \Delta t} \quad (2.2.62b)$$

$$\mathbf{S}_p^{n+1} = e^{-\nu_p \Delta t} \mathbf{S}_p^n + \frac{\epsilon_0 \Delta t \omega_p^2}{\nu_p} e^{-\nu_p \Delta t} \mathbf{E}^{n+1}, \quad \forall p \quad (2.2.62c)$$

$$\mathbf{I}^{n+1} = \mathbf{I}^n + \left(\sum_p \frac{\epsilon_0 \Delta t \omega_p^2}{\nu_p} + \sigma \Delta t \right) \mathbf{E}^{n+1} \quad (2.2.62d)$$

2.3 ADI-FDTD Method

References [3] and [4] first reported the development of ADI-FDTD method which has unconditional stability feature. Since then, it has gained much prominence due to the fact that the time step is no longer restricted by the CFL constraint and simulation time can be further accelerated. While electric and magnetic fields are also staggered in Yee's cell, the six field components are collocated in time instead of staggered, which renders the ADI-FDTD method an implicit algorithm. In the following, the ADI-FDTD method for lossy media as well as its extensions to dispersive media shall be reviewed.

2.3.1 For Lossy Media

The update equation for ADI-FDTD method can be written in compact matrix form as

$$\left(\mathbf{I}_6 - \frac{\Delta t}{2} \mathbf{A} + \frac{\Delta t}{4} \mathbf{L} \right) \mathbf{u}^{n+\frac{1}{2}} = \left(\mathbf{I}_6 + \frac{\Delta t}{2} \mathbf{B} - \frac{\Delta t}{4} \mathbf{L} \right) \mathbf{u}^n \quad (2.3.1a)$$

$$\left(\mathbf{I}_6 - \frac{\Delta t}{2} \mathbf{B} + \frac{\Delta t}{4} \mathbf{L} \right) \mathbf{u}^{n+1} = \left(\mathbf{I}_6 + \frac{\Delta t}{2} \mathbf{A} - \frac{\Delta t}{4} \mathbf{L} \right) \mathbf{u}^{n+\frac{1}{2}} \quad (2.3.1b)$$

where

$$\mathbf{u} = [E_x, E_y, E_z, H_x, H_y, H_z]^T \quad (2.3.2)$$

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{1}{\epsilon}\partial_y \\ 0 & 0 & 0 & \frac{1}{\epsilon}\partial_z & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\epsilon}\partial_x & 0 \\ 0 & \frac{1}{\mu}\partial_z & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\mu}\partial_x & 0 & 0 & 0 \\ \frac{1}{\mu}\partial_y & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (2.3.3)$$

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{-1}{\epsilon}\partial_z & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{-1}{\epsilon}\partial_x \\ 0 & 0 & 0 & \frac{-1}{\epsilon}\partial_y & 0 & 0 \\ 0 & 0 & \frac{-1}{\mu}\partial_y & 0 & 0 & 0 \\ \frac{-1}{\mu}\partial_z & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-1}{\mu}\partial_x & 0 & 0 & 0 & 0 \end{bmatrix} \quad (2.3.4)$$

$$\mathbf{L} = \text{diag} \left(\left[\frac{\sigma}{\epsilon}, \frac{\sigma}{\epsilon}, \frac{\sigma}{\epsilon}, \frac{\sigma^*}{\mu}, \frac{\sigma^*}{\mu}, \frac{\sigma^*}{\mu} \right] \right) \quad (2.3.5)$$

$\mathbf{I}_6$ is the 6×6 identity matrix. ∂_x , ∂_y and ∂_z are the spatial differential operator in x , y and z -directions, respectively. Note that the ADI-FDTD method consists of two substeps (from n to $n + \frac{1}{2}$ and $n + \frac{1}{2}$ to $n + 1$ time steps).

Expanding (2.3.1), upon some manipulations and arrangements, the full update equation of ADI-FDTD method reads:

For first substep n to $n + \frac{1}{2}$:

$$\begin{aligned} & -\frac{c_2 d_2}{\Delta y^2} E_x|_{i+\frac{1}{2}, j-1, k}^{n+\frac{1}{2}} + \left(1 + \frac{2c_2 d_2}{\Delta y^2}\right) E_x|_{i+\frac{1}{2}, j, k}^{n+\frac{1}{2}} - \frac{c_2 d_2}{\Delta y^2} E_x|_{i+\frac{1}{2}, j+1, k}^{n+\frac{1}{2}} \\ & = E_x|_{i+\frac{1}{2}, j, k}^n + \frac{c_2 d_1}{\Delta y} \left(H_z|_{i+\frac{1}{2}, j+\frac{1}{2}, k}^n - H_z|_{i+\frac{1}{2}, j-\frac{1}{2}, k}^n \right) - \frac{c_2}{\Delta z} \left(H_y|_{i+\frac{1}{2}, j, k+\frac{1}{2}}^n - H_y|_{i+\frac{1}{2}, j, k-\frac{1}{2}}^n \right) \\ & \quad - \frac{c_2 d_2}{\Delta y \Delta x} \left(E_y|_{i+1, j+\frac{1}{2}, k}^n - E_y|_{i, j+\frac{1}{2}, k}^n - E_y|_{i+1, j-\frac{1}{2}, k}^n + E_y|_{i, j-\frac{1}{2}, k}^n \right) \\ & - \frac{c_2 d_2}{\Delta z^2} E_y|_{i, j+\frac{1}{2}, k-1}^{n+\frac{1}{2}} + \left(1 + \frac{2c_2 d_2}{\Delta z^2}\right) E_y|_{i, j+\frac{1}{2}, k}^{n+\frac{1}{2}} - \frac{c_2 d_2}{\Delta z^2} E_y|_{i, j+\frac{1}{2}, k+1}^{n+\frac{1}{2}} \\ & = E_y|_{i, j+\frac{1}{2}, k}^n + \frac{c_2 d_1}{\Delta z} \left(H_x|_{i, j+\frac{1}{2}, k+\frac{1}{2}}^n - H_x|_{i, j+\frac{1}{2}, k-\frac{1}{2}}^n \right) - \frac{c_2}{\Delta x} \left(H_z|_{i+\frac{1}{2}, j+\frac{1}{2}, k}^n - H_z|_{i-\frac{1}{2}, j+\frac{1}{2}, k}^n \right) \end{aligned} \quad (2.3.6a)$$

$$- \frac{c_2 d_2}{\Delta z \Delta y} \left(E_z|_{i,j+1,k+\frac{1}{2}}^n - E_z|_{i,j,k+\frac{1}{2}}^n - E_z|_{i,j+1,k-\frac{1}{2}}^n + E_z|_{i,j,k-\frac{1}{2}}^n \right) \quad (2.3.6b)$$

$$\begin{aligned} & - \frac{c_2 d_2}{\Delta x^2} E_z|_{i-1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} + \left(1 + \frac{2c_2 d_2}{\Delta x^2} \right) E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \frac{c_2 d_2}{\Delta x^2} E_z|_{i+1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} \\ & = E_z|_{i,j,k+\frac{1}{2}}^n + \frac{c_2 d_1}{\Delta x} \left(H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n - H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^n \right) - \frac{c_2}{\Delta y} \left(H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n - H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^n \right) \\ & - \frac{c_2 d_2}{\Delta x \Delta z} \left(E_x|_{i+\frac{1}{2},j,k+1}^n - E_x|_{i+\frac{1}{2},j,k}^n - E_x|_{i-\frac{1}{2},j,k+1}^n + E_x|_{i-\frac{1}{2},j,k}^n \right) \end{aligned} \quad (2.3.6c)$$

$$\begin{aligned} H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} & = d_1 H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+} \\ & + d_2 \left(\frac{E_y|_{i,j+\frac{1}{2},k+1}^{n+\frac{1}{2}} - E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta z} - \frac{E_z|_{i,j+1,k+\frac{1}{2}}^n - E_z|_{i,j,k+\frac{1}{2}}^n}{\Delta y} \right) \end{aligned} \quad (2.3.6d)$$

$$\begin{aligned} H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} & = d_1 H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+} \\ & + d_2 \left(\frac{E_z|_{i+1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} - \frac{E_x|_{i+\frac{1}{2},j,k+1}^n - E_x|_{i+\frac{1}{2},j,k}^n}{\Delta z} \right) \end{aligned} \quad (2.3.6e)$$

$$\begin{aligned} H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} & = d_1 H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n \\ & + d_2 \left(\frac{E_x|_{i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}}}{\Delta y} - \frac{E_y|_{i+1,j+\frac{1}{2},k}^n - E_y|_{i,j+\frac{1}{2},k}^n}{\Delta x} \right) \end{aligned} \quad (2.3.6f)$$

For second substep $n + \frac{1}{2}$ to $n + 1$:

$$\begin{aligned} & - \frac{c_2 d_2}{\Delta z^2} E_x|_{i+\frac{1}{2},j,k-1}^{n+1} + \left(1 + \frac{2c_2 d_2}{\Delta z^2} \right) E_x|_{i+\frac{1}{2},j,k}^{n+1} - \frac{c_2 d_2}{\Delta z^2} E_x|_{i+\frac{1}{2},j,k+1}^{n+1} \\ & = E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} + \frac{c_2}{\Delta y} \left(H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - H_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n+\frac{1}{2}} \right) - \frac{c_2 d_1}{\Delta z} \left(H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i+\frac{1}{2},j,k-\frac{1}{2}}^{n+\frac{1}{2}} \right) \\ & - \frac{c_2 d_2}{\Delta z \Delta x} \left(E_z|_{i+1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - E_z|_{i+1,j,k-\frac{1}{2}}^{n+\frac{1}{2}} + E_z|_{i,j,k-\frac{1}{2}}^{n+\frac{1}{2}} \right) \end{aligned} \quad (2.3.7a)$$

$$\begin{aligned} & - \frac{c_2 d_2}{\Delta x^2} E_y|_{i-1,j+\frac{1}{2},k}^{n+1} + \left(1 + \frac{2c_2 d_2}{\Delta x^2} \right) E_y|_{i,j+\frac{1}{2},k}^{n+1} - \frac{c_2 d_2}{\Delta x^2} E_y|_{i+1,j+\frac{1}{2},k}^{n+1} \\ & = E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} + \frac{c_2}{\Delta z} \left(H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n+\frac{1}{2}} \right) - \frac{c_2 d_1}{\Delta x} \left(H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - H_z|_{i-\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} \right) \\ & - \frac{c_2 d_2}{\Delta x \Delta y} \left(E_x|_{i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} - E_x|_{i-\frac{1}{2},j+1,k}^{n+\frac{1}{2}} + E_x|_{i-\frac{1}{2},j,k}^{n+\frac{1}{2}} \right) \end{aligned} \quad (2.3.7b)$$

$$\begin{aligned} & - \frac{c_2 d_2}{\Delta y^2} E_z|_{i,j-1,k+\frac{1}{2}}^{n+1} + \left(1 + \frac{2c_2 d_2}{\Delta y^2} \right) E_z|_{i,j,k+\frac{1}{2}}^{n+1} - \frac{c_2 d_2}{\Delta y^2} E_z|_{i,j+1,k+\frac{1}{2}}^{n+1} \\ & = E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{c_2}{\Delta x} \left(H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} \right) - \frac{c_2 d_1}{\Delta y} \left(H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} \right) \end{aligned}$$

$$- \frac{c_2 d_2}{\Delta y \Delta z} \left(E_y|_{i,j+\frac{1}{2},k+1}^{n+\frac{1}{2}} - E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} - E_y|_{i,j-\frac{1}{2},k+1}^{n+\frac{1}{2}} + E_y|_{i,j-\frac{1}{2},k}^{n+\frac{1}{2}} \right) \quad (2.3.7c)$$

$$H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} = d_1 H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} + d_2 \left(\frac{E_y|_{i,j+\frac{1}{2},k+1}^{n+\frac{1}{2}} - E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta z} - \frac{E_z|_{i,j+1,k+\frac{1}{2}}^{n+1} - E_z|_{i,j,k+\frac{1}{2}}^{n+1}}{\Delta y} \right) \quad (2.3.7d)$$

$$H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+1} = d_1 H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} + d_2 \left(\frac{E_z|_{i+1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} - \frac{E_x|_{i+\frac{1}{2},j,k+1}^{n+1} - E_x|_{i+\frac{1}{2},j,k}^{n+1}}{\Delta z} \right) \quad (2.3.7e)$$

$$H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = d_1 H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} + d_2 \left(\frac{E_x|_{i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}}}{\Delta y} - \frac{E_y|_{i+1,j+\frac{1}{2},k}^{n+1} - E_y|_{i,j+\frac{1}{2},k}^{n+1}}{\Delta x} \right) \quad (2.3.7f)$$

where

$$c_1 = \frac{1 - \frac{\sigma \Delta t}{4\epsilon}}{1 + \frac{\sigma \Delta t}{4\epsilon}}; \quad c_2 = \frac{\frac{\Delta t}{2\epsilon}}{1 + \frac{\sigma \Delta t}{4\epsilon}}; \quad (2.3.8a)$$

$$d_1 = \frac{1 - \frac{\sigma^* \Delta t}{4\mu}}{1 + \frac{\sigma^* \Delta t}{4\mu}}; \quad d_2 = \frac{\frac{\Delta t}{2\mu}}{1 + \frac{\sigma^* \Delta t}{4\mu}}. \quad (2.3.8b)$$

Note that the electric field components are solved implicitly while the magnetic field components are then solved explicitly. In the above, the electric and magnetic fields associated with the electric and magnetic conductivities respectively are averaged between time indices n and $n + \frac{1}{2}$ for the first substep, and $n + \frac{1}{2}$ and $n + 1$ for the second substep. This scheme is commonly known as the averaging scheme [47–49]. There are also other possible schemes of incorporating the electric and magnetic conductivities [50–53]. Some of the common schemes will be further elaborated in Chapter 4. Note that apart from the ADI-FDTD method, there are other implicit methods which also have unconditionally stable feature such as the Locally-One-Dimensional FDTD (LOD-FDTD) method [54, 55] and Crank-Nicholson based implicit FDTD (CN-FDTD) methods [56–59] but they shall not be discussed further

in the thesis.

As for electromagnetic wave source generation in ADI-FDTD method, hard sources are much more difficult to set up due to the implicit nature of the algorithm and thus, seldomly used. The proper use of direct $\mathbf{J}$ and $\mathbf{M}$ sources in ADI-FDTD method are further discussed in [60–65]. The TF/SF formulation for plane wave source condition in ADI-FDTD method has also been presented in [66]. On top of that, the PML has been extended for its usage in ADI-FDTD method [67–70].

2.3.2 Extensions to Dispersive Media

The ADI-FDTD method has also been extended into linear dispersive media [71–76]. In the following, we shall provide the ADI-FDTD method formulation for Debye media using the ADE scheme discussed earlier due to its popularity. The basic concept is to incorporate the auxiliary equations and to update them in synchronism with the implicit update equations of ADI-FDTD for two substeps. For convenience, the subscript indices for all fields are omitted.

For E_x field component of the first substep from n to $n + \frac{1}{2}$, we insert J_{xp} into its update equation in Ampere's law of Maxwell's curl equations to yield

$$\frac{E_x^{n+\frac{1}{2}} - E_x^n}{\Delta t/2} = \frac{1}{\epsilon_0 \epsilon_\infty} \left(\frac{\partial}{\partial y} H_z^{n+\frac{1}{2}} - \frac{\partial}{\partial z} H_y^n - \sigma \frac{E_x^n + E_x^{n+\frac{1}{2}}}{2} - \sum_p \frac{J_{xp}^n + J_{xp}^{n+\frac{1}{2}}}{2} \right). \quad (2.3.9)$$

The J_{xp} field update equation has similar form as those found in the Yee's explicit FDTD method:

$$J_{xp}^{n+\frac{1}{2}} = k_{1p} J_{xp}^n + k_{2p} \left(\frac{E_x^{n+\frac{1}{2}} - E_x^n}{\Delta t/2} \right) \quad (2.3.10)$$

where

$$k_{1p} = \frac{1 - \Delta t/4\tau_p}{1 + \Delta t/4\tau_p}; \quad k_{2p} = \frac{\epsilon_0 \Delta \epsilon_p \Delta t/2\tau_p}{1 + \Delta t/2\tau_p} \quad (2.3.11)$$

Note that the time step of Δt used in Yee's explicit FDTD method are now replaced with $\Delta t/2$ to accomodate for the two-substep nature of the ADI-FDTD method.

Similarly, for E_x field component of the second substep from $n + \frac{1}{2}$ to $n + 1$:

$$\frac{E_x^{n+1} - E_x^{n+\frac{1}{2}}}{\Delta t/2} = \frac{1}{\epsilon_0 \epsilon_\infty} \left(\frac{\partial}{\partial y} H_z^{n+\frac{1}{2}} - \frac{\partial}{\partial z} H_y^{n+1} - \sigma \frac{E_x^{n+\frac{1}{2}} + E_x^{n+1}}{2} - \sum_p \frac{J_{xp}^{n+\frac{1}{2}} + J_{xp}^{n+1}}{2} \right) \quad (2.3.12)$$

in which

$$J_{xp}^{n+1} = k_{1p} J_{xp}^{n+\frac{1}{2}} + k_{2p} \left(\frac{E_x^{n+1} - E_x^{n+\frac{1}{2}}}{\Delta t/2} \right) \quad (2.3.13)$$

To update (2.3.10) and (2.3.13) in synchronism with (2.3.9) and (2.3.12) for the first and second substeps respectively, we again utilize the semi-implicit approximation

$$\frac{1}{2} \left(\mathbf{J}_p^n + \mathbf{J}_p^{n+\frac{1}{2}} \right) = \frac{1}{2} \left[(1 + k_{1p}) \mathbf{J}_p^n + \frac{k_{2p}}{\Delta t/2} (\mathbf{E}^{n+\frac{1}{2}} - \mathbf{E}^n) \right] \quad (2.3.14)$$

and

$$\frac{1}{2} \left(\mathbf{J}_p^{n+\frac{1}{2}} + \mathbf{J}_p^{n+1} \right) = \frac{1}{2} \left[(1 + k_{1p}) \mathbf{J}_p^{n+\frac{1}{2}} + \frac{k_{2p}}{\Delta t/2} (\mathbf{E}^{n+1} - \mathbf{E}^{n+\frac{1}{2}}) \right]. \quad (2.3.15)$$

Upon collecting like terms, and repeating similar procedures to other field componenets, we obtain the full update equation of ADI-FDTD method for Debye media:

For first substep n to $n + \frac{1}{2}$:

$$E_x^{n+\frac{1}{2}} = c_1 E_x^n + c_2 \left(\frac{\partial}{\partial y} H_z^{n+\frac{1}{2}} - \frac{\partial}{\partial z} H_y^n - \frac{1}{2} \sum_p (1 + k_{1p}) J_{xp}^n \right) \quad (2.3.16a)$$

$$E_y^{n+\frac{1}{2}} = c_1 E_y^n + c_2 \left(\frac{\partial}{\partial z} H_x^{n+\frac{1}{2}} - \frac{\partial}{\partial x} H_z^n - \frac{1}{2} \sum_p (1 + k_{1p}) J_{yp}^n \right) \quad (2.3.16b)$$

$$E_z^{n+\frac{1}{2}} = c_1 E_z^n + c_2 \left(\frac{\partial}{\partial x} H_y^{n+\frac{1}{2}} - \frac{\partial}{\partial y} H_x^n - \frac{1}{2} \sum_p (1 + k_{1p}) J_{zp}^n \right) \quad (2.3.16c)$$

$$J_{xp}^{n+\frac{1}{2}} = k_{1p}J_{xp}^n + k_{2p}\left(\frac{E_x^{n+\frac{1}{2}} - E_x^n}{\Delta t/2}\right) \quad (2.3.16d)$$

$$J_{yp}^{n+\frac{1}{2}} = k_{1p}J_{yp}^n + k_{2p}\left(\frac{E_y^{n+\frac{1}{2}} - E_y^n}{\Delta t/2}\right) \quad (2.3.16e)$$

$$J_{zp}^{n+\frac{1}{2}} = k_{1p}J_{zp}^n + k_{2p}\left(\frac{E_z^{n+\frac{1}{2}} - E_z^n}{\Delta t/2}\right) \quad (2.3.16f)$$

$$H_x^{n+\frac{1}{2}} = d_1H_x^n + d_2\left(\frac{\partial}{\partial z}E_y^{n+\frac{1}{2}} - \frac{\partial}{\partial y}E_z^n\right) \quad (2.3.16g)$$

$$H_y^{n+\frac{1}{2}} = d_1H_y^n + d_2\left(\frac{\partial}{\partial x}E_z^{n+\frac{1}{2}} - \frac{\partial}{\partial z}E_x^n\right) \quad (2.3.16h)$$

$$H_z^{n+\frac{1}{2}} = d_1H_z^n + d_2\left(\frac{\partial}{\partial y}E_x^{n+\frac{1}{2}} - \frac{\partial}{\partial x}E_y^n\right) \quad (2.3.16i)$$

For second substep $n + \frac{1}{2}$ to $n + 1$:

$$E_x^{n+1} = c_1E_x^{n+\frac{1}{2}} + c_2\left(\frac{\partial}{\partial y}H_z^{n+\frac{1}{2}} - \frac{\partial}{\partial z}H_y^{n+1} - \frac{1}{2}\sum_p(1+k_{1p})J_{xp}^{n+\frac{1}{2}}\right) \quad (2.3.17a)$$

$$E_y^{n+1} = c_1E_y^{n+\frac{1}{2}} + c_2\left(\frac{\partial}{\partial z}H_x^{n+\frac{1}{2}} - \frac{\partial}{\partial x}H_z^{n+1} - \frac{1}{2}\sum_p(1+k_{1p})J_{yp}^{n+\frac{1}{2}}\right) \quad (2.3.17b)$$

$$E_z^{n+1} = c_1E_z^{n+\frac{1}{2}} + c_2\left(\frac{\partial}{\partial x}H_y^{n+\frac{1}{2}} - \frac{\partial}{\partial y}H_x^{n+1} - \frac{1}{2}\sum_p(1+k_{1p})J_{zp}^{n+\frac{1}{2}}\right) \quad (2.3.17c)$$

$$J_{xp}^{n+1} = k_{1p}J_{xp}^{n+\frac{1}{2}} + k_{2p}\left(\frac{E_x^{n+1} - E_x^{n+\frac{1}{2}}}{\Delta t/2}\right) \quad (2.3.17d)$$

$$J_{yp}^{n+1} = k_{1p}J_{yp}^{n+\frac{1}{2}} + k_{2p}\left(\frac{E_y^{n+1} - E_y^{n+\frac{1}{2}}}{\Delta t/2}\right) \quad (2.3.17e)$$

$$J_{zp}^{n+1} = k_{1p}J_{zp}^{n+\frac{1}{2}} + k_{2p}\left(\frac{E_z^{n+1} - E_z^{n+\frac{1}{2}}}{\Delta t/2}\right) \quad (2.3.17f)$$

$$H_x^{n+1} = d_1H_x^{n+\frac{1}{2}} + d_2\left(\frac{\partial}{\partial z}E_y^{n+\frac{1}{2}} - \frac{\partial}{\partial y}E_z^{n+1}\right) \quad (2.3.17g)$$

$$H_y^{n+1} = d_1H_y^{n+\frac{1}{2}} + d_2\left(\frac{\partial}{\partial x}E_z^{n+\frac{1}{2}} - \frac{\partial}{\partial z}E_x^{n+1}\right) \quad (2.3.17h)$$

$$H_z^{n+1} = d_1H_z^{n+\frac{1}{2}} + d_2\left(\frac{\partial}{\partial y}E_x^{n+\frac{1}{2}} - \frac{\partial}{\partial x}E_y^{n+1}\right) \quad (2.3.17i)$$

where

$$c_1 = \frac{1 - \frac{\sigma \Delta t}{4\epsilon_0 \epsilon_\infty} + \frac{\Delta t}{4\epsilon_0 \epsilon_\infty} \sum_p k_{2p}}{1 + \frac{\sigma \Delta t}{4\epsilon} + \frac{\Delta t}{4\epsilon_0 \epsilon_\infty} \sum_p k_{2p}}; \quad c_2 = \frac{\frac{\Delta t}{2\epsilon_0 \epsilon_\infty}}{1 + \frac{\sigma \Delta t}{4\epsilon_0 \epsilon_\infty} + \frac{\Delta t}{4\epsilon_0 \epsilon_\infty} \sum_p k_{2p}}; \quad (2.3.18a)$$

$$d_1 = \frac{1 - \frac{\sigma^* \Delta t}{4\mu}}{1 + \frac{\sigma^* \Delta t}{4\mu}}; \quad d_2 = \frac{\frac{\Delta t}{2\mu}}{1 + \frac{\sigma^* \Delta t}{4\mu}}. \quad (2.3.18b)$$

Similar to previous chapter, to solve for E fields implicitly, the update equations of the H fields in both substeps are substituted to the respective E fields equations. J fields and H fields are then updated explicitly after the values of E fields are obtained. The formulation for Lorentz and Drude media [75] are straight forward and can be carried out easily in a similar fashion. Other formulation schemes based the PLRC and Z-transform methods are also possible and have been attempted in [74, 76].

2.4 Stability and Dispersion Analysis

For stability analysis, the well known von Neumann method [77] is usually adopted due to its simplicity. In this method, the solutions of a monochromatic plane wave traveling along positive x , y , and z directions are first assumed. Upon applying to all the fields in the Yee's cell, one will arrive at the following

$$E_x|_{I+\frac{1}{2},J,K}^n = \tilde{E}_{x0} e^{j(\omega n \Delta t - k_x(I+\frac{1}{2})\Delta x - k_y J \Delta y - k_z K \Delta z)} \quad (2.4.1a)$$

$$E_y|_{I,J+\frac{1}{2},K}^n = \tilde{E}_{y0} e^{j(\omega n \Delta t - k_x I \Delta x - k_y(J+\frac{1}{2})\Delta y - k_z K \Delta z)} \quad (2.4.1b)$$

$$E_z|_{I,J,K+\frac{1}{2}}^n = \tilde{E}_{z0} e^{j(\omega n \Delta t - k_x I \Delta x - k_y J \Delta y - k_z(K+\frac{1}{2})\Delta z)} \quad (2.4.1c)$$

$$H_x|_{I,J+\frac{1}{2},K+\frac{1}{2}}^n = \tilde{H}_{x0} e^{j(\omega n \Delta t - k_x I \Delta x - k_y(J+\frac{1}{2})\Delta y - k_z(K+\frac{1}{2})\Delta z)} \quad (2.4.1d)$$

$$H_y|_{I+\frac{1}{2},J,K+\frac{1}{2}}^n = \tilde{H}_{y0} e^{j(\omega n \Delta t - k_x(I+\frac{1}{2})\Delta x - k_y J \Delta y - k_z(K+\frac{1}{2})\Delta z)} \quad (2.4.1e)$$

$$H_z|_{I+\frac{1}{2},J+\frac{1}{2},K}^n = \tilde{H}_{z0} e^{j(\omega n \Delta t - k_x(I+\frac{1}{2})\Delta x - k_y(J+\frac{1}{2})\Delta y - k_z K \Delta z)} \quad (2.4.1f)$$

where k_x , k_y and k_z are the wave numbers along the x , y , and z directions. Note that the spatial indices of the fields in this section are written in the form of I , J and K to avoid confusion with wave numbers and $j = \sqrt{-1}$.

In Yee's explicit FDTD method, by utilizing the above relations, a detailed proof of the derivation of the CFL constraint was provided in [6] by solving a pair of eigenvalue problems. The CFL condition is given by

$$\Delta t \leq \sqrt{\frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}. \quad (2.4.2)$$

It can be seen that the maximum allowed time step is restricted by the smallest cell size used. In some structures where there are combinations of fine and coarse grids, the time step is always restricted to the size of the fine grids, which degrades the efficiency significantly. Some stability analysis on nondispersive and lossy media for Yee's explicit FDTD method can be found in [78–80]. For dispersive media, some numerical stability analysis have been performed [81, 82]. To further obtain the stability criterion analytically, the von Neumann method can be combined with the Routh-Hurwitz criteria [83, 84].

On the other hand, the ADI-FDTD method has the advantage of unconditional stability which allows the time step to be selected at a larger value, thus enables the time marching to be accelerated to improve efficiency. Unconditionally stable methods therefore offer a better trade-off between the accuracy and efficiency. The analytical proof of unconditional stability of ADI-FDTD was provided in [3]. Again using the von Neumann method, the updating procedure of the ADI-FDTD method can be represented in a matrix form as

$$\tilde{\mathbf{u}}^{n+1} = \mathbf{\Lambda} \cdot \tilde{\mathbf{u}}^n \quad (2.4.3)$$

where $\tilde{\mathbf{u}} = [\tilde{E}_{x_0}, \tilde{E}_{y_0}, \tilde{E}_{z_0}, \tilde{H}_{x_0}, \tilde{H}_{y_0}, \tilde{H}_{z_0}]^T$ and $\mathbf{\Lambda}$ is the updating matrix. Uncondi-

tional stability is ensured if all the eigenvalues are of magnitude one and at the same time, independent of the time steps and cell size. In ADI-FDTD method, the energy method [49, 85, 86] has also been widely used as an alternative method to the Von Neumann eigenvalue approach. In addition, the stability analysis of ADI-FDTD method can also be performed by means of matrix norm approach [87, 88].

The dispersion relation, on the other hand, describes the variation between propagating wave's phase velocity v and frequency f . Dispersion can also be represented as the variation of propagating wave's wavenumber $k = 2\pi/\lambda$ with angular frequency $\omega = 2\pi f$ where λ is the medium wavelength. The analytical dispersion relation for a plane wave propagating in a continuous medium is expressed as

$$\left(\frac{\omega}{v}\right)^2 = k_x^2 + k_y^2 + k_z^2. \quad (2.4.4)$$

In FDTD grid where the space is discretized into a Yee's cell, the phase velocity of the numerical wave in the FDTD grid no longer stays the same as in continuous medium. It can vary according to vacuum speed of light, wavelength, direction of propagation and grid size. This dispersion caused by the discretization of grids is called the numerical dispersion. The dispersion relation of a particular time stepping method can be obtained by first considering

$$\left(e^{j\omega\Delta t}\mathbf{I}_6 - \mathbf{\Lambda}\right) \tilde{\mathbf{u}}^n. \quad (2.4.5)$$

For nontrivial solution of (2.4.5), the dispersion relation can be derived by setting

$$\det\left(e^{j\omega\Delta t}\mathbf{I}_6 - \mathbf{\Lambda}\right) = 0 \quad (2.4.6)$$

Since the stability and dispersion analysis always originated from the update procedures matrix, the analysis is closely associated to each other and usually they are performed together. Some accuracy and dispersion analysis of Yee's explicit FDTD

method have been reported in [89–93], while the related works on the ADI-FDTD method can be found in [94–103].

Chapter 3

Yee's Explicit FDTD Method for Lossy and Dispersive Media

3.1 Introduction

The effects of lossy media and conductors have been treated by incorporating the conductivity into the original formulation of lossless FDTD update equations. By far, there are four known schemes for such purposes. One common scheme is the time-average (TA) [2]. Other variants include the time-forward (TF) [5], time-backward (TB) [6] and the exponential time differencing (ETD) [7,8]. The stability criterion of FDTD scheme in lossless media was first shown in [6]. Following that, in [78,79], the stability analysis for TA, TF and TB was shown in 3-D, while the stability criterion for ETD was derived only for 1-D in [80]. Using transformation method, a new stability criterion was further developed in [8] for ETD in 3-D under the PML matching condition ($\sigma/\epsilon = \sigma^*/\mu$). The past literatures on stability analysis for Yee's explicit FDTD method are summarized in Table 3.1.

In all the above mentioned works, the stability analysis is performed either for only electrically lossy media ($\sigma^* = 0$), or PML matching condition. Moreover, the stability criterion obtained is only restricted to a particular scheme and not easily applicable to other different schemes or magnetically lossy media. For instance, the

Table 3.1: Past literatures on stability analysis for Yee's explicit FDTD method.

Scheme		Literatures
Doubly Lossy	ETD	[8], only for $\sigma/\epsilon = \sigma^*/\mu$
	TA	None
	TF	None
	TB	None
Electrically Lossy ($\sigma^* = 0$)	ETD	[80], only for 1-D
	TA	[78, 79]
	TF	[79]
	TB	[79]
Lossless		[6]

generalized stability criterion obtained in [79] for electrically lossy media is applicable for weighted average related schemes such as TA, TF or TB. However, finding the stability criterion for ETD remains elusive. More importantly, we are interested to find the stability criterion for the most general case of doubly lossy media where both electric and magnetic conductivities coexist (i.e. $\sigma \neq 0, \sigma^* \neq 0$). Furthermore, the dispersion analysis of TA in [93] had been confined to only electrically lossy media, and it is often desirable to carry out the investigation for the more general doubly lossy media, where both electric and magnetic conductivities are nonzero. For instance, the media used for PML [13] as absorbing boundary conditions require nonzero electric and magnetic conductivities. Certain ferrite composites [104, 105], magnetic materials [106] and wave absorbers [107, 108] are also known to possess both electric and magnetic loss tangents, which find many applications in microwave engineering.

In this chapter, we present the generalized stability criterion of 3-D Yee's explicit FDTD schemes for doubly lossy media. The stability criterion is expressed in terms of generalized update coefficients and thus, applicable for all aforementioned

schemes. Furthermore, it is reducible to the case of either electrically lossy, magnetically lossy or even lossless media. The stability criterion for PML matching condition can also be obtained as a special case to the doubly lossy media. We also present the 3-D dispersion analysis of Yee's explicit FDTD schemes for doubly lossy media, with more emphasis being placed on ETD, TA and TF. The lossless CFL limit will be applied for fair comparison, while time step used beyond the lossless CFL limit is beyond the scope of this chapter.

Chapter 2 has provided a review of numerous efforts carried out to extend the Yee's explicit FDTD method for dispersive media. To briefly name a few here, one approach is the ADE method (or Direct Integration method) [31–36], which converts the frequency-dependent Maxwell equations into auxiliary differential equations in time domain. An alternative approach is by discretizing the convolution integral relating the D and E fields, which results in RC method [25,26] and PLRC method [27]. In [37,38], a Z-transform method was proposed which converts the transfer function in frequency domain into Z domain via a table of conversion. With this approach, the update equations can be obtained much more conveniently than the RC and PLRC methods. On the other hand, the Z-transform method in [40,41] utilizes a single pole conductivity model to incorporate the dispersive effect of material under consideration. This is a distinct method that is not based on frequency domain but Z domain transfer function directly, and thus it will not be considered further in this chapter.

The Z-transform method of [37,38] is in fact the classical impulse invariance method widely used in digital IIR filter design. This method, however, is incorrect and inaccurate when the impulse response is discontinuous at initial time $t = 0$. The problem had been highlighted in [111,112] along with the necessary correction for it. Therefore, if classical impulse invariance method is to be used without any

correction to formulate the FDTD update equations for dispersive media, the overall accuracy of the computed electric and magnetic fields would be affected. It had been previously demonstrated in [113] that using the corrected impulse invariance method to model dispersive media would achieve an improved accuracy to the calculated electric fields. In this chapter, we present the thorough discussions of corrected impulse invariance method in the realm of Z transform theory for dispersive media. A Z-transform table is provided to supplement and *correct* those Z-transform tables provided in [37,38]. With the aid of the table, various formulations of FDTD update equations for dispersive media are carried out conveniently. Detailed performance measures such as numerical permittivity, leading error term, dispersion relation, normalized phase and attenuation errors as well as memory storage requirements are included along with some extensive numerical comparisons.

3.2 Yee's Explicit FDTD Schemes for Doubly Lossy Media

Consider a source-free, isotropic, homogeneous doubly lossy medium. Recall the Maxwell's curl equations in differential form:

$$\epsilon \frac{\partial}{\partial t} \mathbf{E} - \sigma \mathbf{E} = \nabla \times \mathbf{H} \quad (3.2.1a)$$

$$\mu \frac{\partial}{\partial t} \mathbf{H} - \sigma^* \mathbf{H} = -\nabla \times \mathbf{E} \quad (3.2.1b)$$

Note that in practice, second-order central differencing is usually adopted for spatial derivatives (curl) in (3.2.1) and all fields are properly staggered on a Yee's cell. On the other hand, different ways of discretizing (3.2.1) in time will give rise to different schemes. For discretization of Ampere's law (3.2.1a), we begin by expressing the

exact solution to the first-order differential equation (3.2.1a) as

$$\mathbf{E}(t) = e^{-\frac{(t-t_0)}{\tau}} \mathbf{E}(t_0) + \frac{1}{\epsilon} \int_{t_0}^t e^{-\frac{(t-t')}{\tau}} \left(\nabla \times \mathbf{H}(t') \right) dt' \quad (3.2.2)$$

where t_0 is the initial time and $\tau = \epsilon/\sigma$. The generalized update equation of FDTD schemes for electric field can be written as

$$\mathbf{E}^{n+1} = c_1 \mathbf{E}^n + c_2 \nabla \times \mathbf{H}^{n+\frac{1}{2}} \quad (3.2.3)$$

where c_1 and c_2 are the electric field update coefficients.

The electric field update coefficients for ETD, TA, TF and TB are given as follows:

$$\text{ETD: } c_1^{ETD} = e^{-\frac{\Delta t}{\tau}}, \quad c_2^{ETD} = \frac{1 - e^{-\frac{\Delta t}{\tau}}}{\sigma}$$

$$\text{TA: } c_1^{TA} = \frac{1 - \frac{\Delta t}{2\tau}}{1 + \frac{\Delta t}{2\tau}}, \quad c_2^{TA} = \frac{\Delta t/\epsilon}{1 + \frac{\Delta t}{2\tau}}$$

$$\text{TF: } c_1^{TF} = \frac{1}{1 + \frac{\Delta t}{\tau}}, \quad c_2^{TF} = \frac{\Delta t/\epsilon}{1 + \frac{\Delta t}{\tau}}$$

$$\text{TB: } c_1^{TB} = 1 - \frac{\Delta t}{\tau}, \quad c_2^{TB} = \frac{\Delta t}{\epsilon}$$

We first note that the update coefficients of ETD are the closest compared to the analytical solution (3.2.1a). In fact, it should also be pointed out that by applying the following second-order Pade approximation to the ETD update coefficients,

$$e^{-t} = \frac{1 - t/2}{1 + t/2} + O(t^3) \quad (3.2.4)$$

we will recover the TA update coefficients. Therefore, TA is a further Pade approximation of the ETD scheme, though both schemes still maintain overall temporal

accuracy of second-order. On the other hand, TF utilizes forward differencing for its time derivative and TB utilizes backward differencing, which result in only first-order accuracy in time.

For doubly lossy media, the discretization of Faraday's law (3.2.1b) follows in the similar manner. The generalized update equation for magnetic field is given as

$$\mathbf{H}^{n+\frac{3}{2}} = d_1 \mathbf{H}^{n+\frac{1}{2}} - d_2 \nabla \times \mathbf{E}^{n+1} \quad (3.2.5)$$

The magnetic field update coefficients d_1 and d_2 for all the schemes can then be obtained by replacing τ , ϵ , and σ in the previous electric field update coefficients with τ^* , μ , and σ^* , respectively, where $\tau^* = \mu/\sigma^*$.

3.3 Generalized Stability Criterion for Doubly Lossy Media

Using von-Neumann analysis and normalized fields components $\mathbf{e} = \sqrt{\epsilon}\mathbf{E}$ and $\mathbf{h} = \sqrt{\mu}\mathbf{H}$, we can cast the whole update equations of 3-D FDTD schemes for doubly lossy media into

$$\mathbf{u}^{n+1} = (\mathbf{I}_6 - \mathbf{B})^{-1}(\mathbf{D} + \mathbf{A})\mathbf{u}^n = \mathbf{M}\mathbf{u}^n \quad (3.3.1)$$

where

$$\mathbf{u} = [e_x, e_y, e_z, h_x, h_y, h_z]^T \quad (3.3.2)$$

$$\mathbf{A} = c_2 \begin{bmatrix} \mathbf{O}_3 & \mathbf{O}_3 \\ -\mathbf{C} & \mathbf{O}_3 \end{bmatrix} \quad \mathbf{B} = d_2 \begin{bmatrix} \mathbf{O}_3 & \mathbf{C} \\ \mathbf{O}_3 & \mathbf{O}_3 \end{bmatrix} \quad (3.3.3)$$

$$\mathbf{C} = \frac{1}{\sqrt{\mu\epsilon}} \begin{bmatrix} 0 & jK_z & -jK_y \\ -jK_z & 0 & jK_x \\ jK_y & -jK_x & 0 \end{bmatrix} \quad (3.3.4)$$

$$\mathbf{D} = \begin{bmatrix} c_1 \mathbf{I}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & d_1 \mathbf{I}_3 \end{bmatrix} \quad (3.3.5)$$

$$K_\xi = 2 \sin(k_\xi \Delta\xi/2) / \Delta\xi \quad (3.3.6)$$

c_1, c_2 are the generalized update coefficients for normalized electric fields, and their dual d_1, d_2 are for normalized magnetic fields. These generalized update coefficients include nonzero σ and σ^* for doubly lossy media, and will be provided later for different FDTD schemes. k_ξ and $\Delta\xi$ are the wavenumbers and spatial steps in x , y and z directions respectively. $\mathbf{I}_r$ and $\mathbf{O}_r$ are the identity and null matrices with dimensions $r \times r$, respectively. The eigenvalues of the overall updating matrix $\mathbf{M}$ can be solved as

$$\lambda_1 = c_1, \quad \lambda_2 = d_1, \quad (3.3.7)$$

$$\lambda_3 = \lambda_4 = p + q, \quad (3.3.8)$$

$$\lambda_5 = \lambda_6 = p - q \quad (3.3.9)$$

where

$$p = \frac{1}{2}(c_1 + d_1) - \frac{1}{2}c_2 d_2 W^2 \quad (3.3.10)$$

$$q = \frac{1}{2}\sqrt{(W^2 - r_+)(W^2 - r_-)} \quad (3.3.11)$$

$$W^2 = \frac{1}{\mu\epsilon}(K_x^2 + K_y^2 + K_z^2) \quad (3.3.12)$$

$$r_\pm = \frac{c_1 + d_1 \pm 2\sqrt{c_1 d_1}}{c_2 d_2} \quad (3.3.13)$$

For stable algorithm, all magnitudes of eigenvalues have to be less than or equal to one, $|\lambda_i| \leq 1$. From the first two eigenvalues, we obtain

$$|c_1| \leq 1, \quad |d_1| \leq 1 \quad (3.3.14)$$

For the remaining eigenvalues, we note that q can only be either positively real or

purely imaginary. Consider these two possibilities separately. When q is purely imaginary, we find that two complex-conjugate pairs of eigenvalues exist, with magnitudes

$$|\lambda_3| = |\lambda_4| = |\lambda_5| = |\lambda_6| = \sqrt{c_1 d_1} \quad (3.3.15)$$

If (3.3.14) holds, then $\sqrt{c_1 d_1} \leq 1$ and the stability for purely imaginary q is guaranteed.

On the other hand, to ensure stability for positive real q , we ought to have

$$-1 \leq p - q \leq p + q \leq 1 \quad (3.3.16)$$

along with (3.3.14). It can be shown, upon some manipulations that (3.3.16) is satisfied if and only if

$$\frac{c_1 + d_1 - c_1 d_1 - 1}{c_2 d_2} \leq W^2 \leq \frac{1 + c_1 + d_1 + c_1 d_1}{c_2 d_2} \quad (3.3.17)$$

Since (3.3.14) holds, we find that

$$\frac{c_1 + d_1 - c_1 d_1 - 1}{c_2 d_2} \leq 0 \quad (3.3.18)$$

For nonnegative W^2 , (3.3.17) can be further reduced into

$$W^2 \leq \frac{1 + c_1 + d_1 + c_1 d_1}{c_2 d_2} \quad (3.3.19)$$

The overall necessary and sufficient condition to guarantee algorithm stability for all q is therefore given by

$$|c_1| \leq 1, \quad |d_1| \leq 1 \quad (3.3.20a)$$

$$\frac{4c_2 d_2}{1 + c_1 + d_1 + c_1 d_1} \leq \frac{\mu \epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}} \quad (3.3.20b)$$

Equation (3.3.20) represents the generalized stability criterion of 3-D FDTD schemes

for doubly lossy media. This generalized stability criterion is very versatile and convenient in a sense that, for any particular scheme, one would only need to replace c_1 , c_2 , d_1 and d_2 with their corresponding update coefficients.

Table 3.2: Stability criterion and update coefficients for 3-D FDTD schemes. ©2010 IEEE.

Scheme		c_1	c_2	d_1	d_2	Stability Criterion
Doubly Lossy	ETD	$e^{-\frac{\Delta t}{\tau}}$	$\tau(1 - e^{-\frac{\Delta t}{\tau}})$	$e^{-\frac{\Delta t}{\tau^*}}$	$\tau^*(1 - e^{-\frac{\Delta t}{\tau^*}})$	$\frac{4\tau\tau^*(1-e^{-\frac{\Delta t}{\tau}})(1-e^{-\frac{\Delta t}{\tau^*}})}{(1+e^{-\frac{\Delta t}{\tau}})(1+e^{-\frac{\Delta t}{\tau^*}})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	TA ($a = \frac{1}{2}, b = \frac{1}{2}$)	$\frac{1 - \frac{\Delta t}{2\tau}}{1 + \frac{\Delta t}{2\tau}}$	$\frac{\Delta t}{1 + \frac{\Delta t}{2\tau}}$	$\frac{1 - \frac{\Delta t}{2\tau^*}}{1 + \frac{\Delta t}{2\tau^*}}$	$\frac{\Delta t}{1 + \frac{\Delta t}{2\tau^*}}$	$\Delta t^2 \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	TF ($a = 1, b = 0$)	$\frac{1}{1 + \frac{\Delta t}{\tau}}$	$\frac{\Delta t}{1 + \frac{\Delta t}{\tau}}$	$\frac{1}{1 + \frac{\Delta t}{\tau^*}}$	$\frac{\Delta t}{1 + \frac{\Delta t}{\tau^*}}$	$\frac{\Delta t^2}{(1 + \frac{\Delta t}{2\tau})(1 + \frac{\Delta t}{2\tau^*})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	TB ($a = 0, b = 1$)	$1 - \frac{\Delta t}{\tau}$	Δt	$1 - \frac{\Delta t}{\tau^*}$	Δt	$\frac{\Delta t \leq 2\min(\tau, \tau^*)}{(1 - \frac{\Delta t}{2\tau})(1 - \frac{\Delta t}{2\tau^*})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	Weighted Average (any $a + b = 1$)	$\frac{1-b}{1+a} \frac{\Delta t}{\tau}$	$\frac{\Delta t}{1+a} \frac{\Delta t}{\tau}$	$\frac{1-b}{1+a} \frac{\Delta t}{\tau^*}$	$\frac{\Delta t}{1+a} \frac{\Delta t}{\tau^*}$	$\frac{(b-a)\Delta t \leq 2\min(\tau, \tau^*)}{(1+(a-b)\frac{\Delta t}{2\tau})(1+(a-b)\frac{\Delta t}{2\tau^*})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
Electrically Lossy ($\sigma^* = 0$)	ETD	$e^{-\frac{\Delta t}{\tau}}$	$\tau(1 - e^{-\frac{\Delta t}{\tau}})$	1	Δt	$\frac{2\tau(1-e^{-\frac{\Delta t}{\tau}})\Delta t}{(1+e^{-\frac{\Delta t}{\tau}})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	TA ($a = \frac{1}{2}, b = \frac{1}{2}$)	$\frac{1 - \frac{\Delta t}{2\tau}}{1 + \frac{\Delta t}{2\tau}}$	$\frac{\Delta t}{1 + \frac{\Delta t}{2\tau}}$			$\Delta t^2 \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	TF ($a = 1, b = 0$)	$\frac{1}{1 + \frac{\Delta t}{\tau}}$	$\frac{\Delta t}{1 + \frac{\Delta t}{\tau}}$			$\frac{\Delta t^2}{(1 + \frac{\Delta t}{2\tau})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	TB ($a = 0, b = 1$)	$1 - \frac{\Delta t}{\tau}$	Δt			$\frac{\Delta t \leq 2\tau}{(1 - \frac{\Delta t}{2\tau})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
	Weighted Average (any $a + b = 1$)	$\frac{1-b}{1+a} \frac{\Delta t}{\tau}$	$\frac{\Delta t}{1+a} \frac{\Delta t}{\tau}$			$\frac{(b-a)\Delta t \leq 2\tau}{(1+(a-b)\frac{\Delta t}{2\tau})} \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$
Lossless ($\sigma = \sigma^* = 0$)		1	Δt	1	Δt	$\Delta t^2 \leq \frac{\mu\epsilon}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$

$$\tau = \epsilon/\sigma, \quad \tau^* = \mu/\sigma^*$$

Table 3.2 provides the stability criterion for 3-D FDTD schemes, as well as their respective update coefficients. For nonnegative Δt , τ and τ^* , the conditions in

(3.3.20a) are redundant for ETD, TA and TF because $|c_1|$ and $|d_1|$ are always less than or equal to absolute one. For TB, $\Delta t \leq 2 \min(\tau, \tau^*)$ and $\Delta t \leq 2\tau$ are needed for doubly lossy and electrically lossy media, respectively, in order to ensure (3.3.20a). This implies that for TB, the time step is not only restricted by the cell size, it also has to sufficiently resolve the minimum relaxation time of the medium, where the electric and magnetic relaxation time are commonly defined as ϵ/σ and μ/σ^* , respectively. Hence, it is anticipated that its stability criterion will be more stringent compared to other schemes, as shall be shown later. For completeness, TA, TF and TB can be further generalized into weighted average scheme, and its entries are also included with coefficients a and b defined in [79]. The stability criterion for 1 or 2-D is very straight forward by removing either one or two of the spatial steps. Three types of media are shown, the doubly lossy, electrically lossy and lossless. The magnetically lossy media are the dual of electrically lossy media, and the stability criterion can be obtained simply by replacing τ with τ^* . The stability criterion of TA, TF, TB and weighted average schemes obtained for electrically lossy media is consistent with those found in [78, 79]. The stability criterion of ETD in Table 3.2 is also consistent with the one found in [80] for 1-D electrically lossy media. Furthermore, we note that the stability criterion (equation (8) in [8]) obtained by transformation method is only applicable for PML matching condition ($\tau = \tau^*$) and belongs to the special case of our generalized doubly lossy ETD scheme.

3.4 Numerical Results for Stability Analysis

It has been shown in previous studies [78–80] that the stability criterion for electrically lossy media remains unchanged for TA, is more relaxed for TF, ETD and is more stringent for TB compared to FDTD scheme in lossless media. Here, we further show that for doubly lossy media, stability criterion for TA still remains

Figure 3.1: 3-D plots of stability factor with respect to $\sigma/\omega\epsilon$ and $\sigma^*/\omega\mu$ for (a) TA, (b) ETD, (c) TF, (d) TB. ©2010 IEEE.

unchanged. For TF and ETD, the stability criterion is even more relaxed than that of electrically lossy media, while it is even more stringent for TB. We first introduce the stability factor, f by bringing all terms in (3.3.20b) to the left hand side:

$$f = \frac{4c_2d_2(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2})}{(1 + c_1 + d_1 + c_1d_1)\mu\epsilon} \quad (3.4.1)$$

The stability factor will serve as a measure as to how stable a particular scheme is at any arbitrary $\Delta x, \Delta y, \Delta z, \Delta t, \tau$ and τ^* . A stability factor larger than one

Figure 3.2: Snapshot of reflected and transmitted electric fields through thin conductor ($\sigma = 10^5 \text{S/m}$, $\sigma^* = 10^5 \Omega/\text{m}$) after 96.5ps. ©2010 IEEE.

indicates instability and vice-versa. Fig. 3.1 shows the 3-D plots of stability factor with respect to $\sigma/\omega\epsilon$ and $\sigma^*/\omega\mu$ for (a) TA, (b) ETD, (c) TF and (d) TB. Uniform cells ($\Delta x = \Delta y = \Delta z$) are assumed and the frequency is arbitrarily fixed at 10 GHz. CPW is set at 10 at that particular frequency and Δt is chosen as the 3-D lossless Courant limit. Note that all these parameters are fixed throughout with only σ and σ^* varied. We observe that for TA, stability factor remains at one throughout, which indicates that the stability criterion is unperturbed by σ, σ^* and is still the same as the lossless case. For ETD and TF, a negative gradient for stability factor is seen with increasing σ and σ^* . This suggests that toward increasing σ and σ^* , both schemes have more increment room for their Δt before reaching instability (i.e. more relaxed criterion). Also, TF has slightly smaller stability factor (slightly more relaxed stability criterion) throughout compared to ETD. On the other hand, we observe a positive gradient for stability factor of TB, which is a clear indication of more stringent criterion toward increasing σ and σ^* .

As numerical demonstration, we simulate the tunneling phenomena of 1-D electro-

Figure 3.3: Instability shown by TA around thin conductor after 1000 iterations (Δt set at maximum allowed Δt of ETD instead of its own). ©2010 IEEE.

Table 3.3: CPU time incurred by different FDTD schemes. ©2010 IEEE.

Scheme	Δt	Total no. of Iterations	CPU Time
TA	8.339×10^{-16}	115711	1.666s
ETD	3.927×10^{-15}	24572	0.353s
TF	4.097×10^{-15}	23550	0.339s

magnetic wave propagation through a very thin conductor with doubly lossy nature. A domain of 150 cells with nonuniform cell size are adopted. Two cells at the centre are filled with a doubly lossy conductor with $\sigma = 10^5 \text{S/m}$, $\sigma^* = 10^5 \Omega/\text{m}$ and the rest are free space. Each cell size of the conductor is set at $0.25 \mu\text{m}$, while for the rest of the cell, cell per wavelength (CPW) is chosen as 10 at 150 GHz. An electric field gaussian pulse $g(t) = \exp\left(-\left(\frac{(t-t_d)}{t_w}\right)^2\right)$ where $t_d = 18.75\text{ps}$, $t_w = 6.25\text{ps}$ is launched at initial point as a hard source impinging upon the conductor, and the simulation is terminated after 96.5ps. Since TB has an even more stringent stability criterion in doubly lossy media compared to TA, it shall be omitted here due to its inefficiency. The experiment is run using three different schemes, TA, ETD and TF with time step, Δt set at their respective maximum allowed time step, listed in Table 3.3.

The maximum allowed time step is solved from the stability criterion in Table 3.2 with minimum cell size $0.25\mu\text{m}$. It can be seen from Table 3.3 that ETD and TF have more relaxed Δt , and therefore, less total number of iterations and CPU time needed for the simulation compared to TA. We can also see that TF has a slightly more relaxed Δt compared to ETD. Fig. 3.2 shows the snapshot of electric fields after 96.5ps. As long as the doubly lossy conductor is sufficiently thin, we observe a portion of electric field being able to tunnel through the thin conductor, and the rest being reflected. Fig. 3.3 further shows the instability exhibited by TA around the thin conductor just after 1000 iterations if Δt is set at ETD's more relaxed Δt instead of its own maximum allowed time step.

To further verify the stability criterion provided in Table 3.2, we consider a $50 \times 50 \times 50$ meshed cavity with PEC walls and uniform cell size of 35mm, being excited by a point current source at the centre. The cavity is filled with doubly lossy medium, where σ and σ^* are arbitrarily set as 0.1S/m and $100\Omega/\text{m}$, respectively. Simulations are performed using the schemes of ETD, TA, TF and TB, with Δt set at their maximum allowed time step as 69.0757ps, 67.4041ps, 81.5990ps and 55.7355ps (solved from Table 3.2), respectively. No instability is observed under such circumstances. The experiments are then repeated, with the respective Δt slightly amplified by a factor of 1.001. In this case, exponential growth of fields originating from the point source are visible as the time marches. These further confirm and ascertain the stability criterion of FDTD schemes derived previously.

Table 3.4: Complex numerical permittivity and leading error term for FDTD schemes

Scheme	Complex Numerical Permittivity	Leading Error Term
ETD	$\frac{\sigma \Delta t e^{j\omega \frac{\Delta t}{2}} (1 - e^{-\Delta t(\frac{1}{\tau} + j\omega)})}{j2 \sin(\omega \frac{\Delta t}{2})(1 - e^{-\frac{\Delta t}{\tau}})}$	$\Delta t^2 (\frac{j\sigma\omega}{12} + \frac{\sigma^2}{12\epsilon})$
TA	$\epsilon + \frac{\sigma \Delta t \cot(\omega \frac{\Delta t}{2})}{2j}$	$\Delta t^2 (\frac{j\sigma\omega}{12})$
TF	$\epsilon + \frac{\sigma \Delta t}{2} + \frac{\sigma \Delta t \cot(\omega \frac{\Delta t}{2})}{2j}$	$\Delta t \frac{\sigma}{2}$
TB	$\epsilon - \frac{\sigma \Delta t}{2} + \frac{\sigma \Delta t \cot(\omega \frac{\Delta t}{2})}{2j}$	$-\Delta t \frac{\sigma}{2}$

3.5 Dispersion Analysis for Doubly Lossy Media

By substituting the Fourier modes to all fields in the update equations detailed in the previous section, one will arrive at the generalized dispersion relation as follows:

$$\sum_{\xi=x,y,z} \left(\frac{2}{\Delta \xi} \sin(k_\xi \Delta \xi / 2) \right)^2 = \left(\frac{2}{\Delta t} \sin(\omega \Delta t / 2) \right)^2 \mu_{nc} \epsilon_{nc} \quad (3.5.1)$$

ϵ_{nc} and μ_{nc} are known as the complex numerical permittivity and permeability which are unique to a particular FDTD scheme in doubly lossy media. Note that in lossless media, $\epsilon_{nc} = \epsilon$, $\mu_{nc} = \mu$ and (3.5.1) will recover the original dispersion relation of FDTD scheme in lossless media. The complex numerical permittivity of each scheme is shown clearly in Table 3.4. Also shown in Table 3.4 is the truncation error term in Δt compared to the analytical complex permittivity in doubly lossy media given by $\epsilon(\omega) = \epsilon - j\frac{\sigma}{\omega}$. On the other hand, complex numerical permeability of each scheme and their respective leading truncation error can be obtained simply by substituting σ , ϵ with σ^* , μ , respectively, and thus, shall not be repeated. For all discretization parameters Δx , Δy , Δz and Δt approaching zero, ϵ_{nc} approaches $\epsilon(\omega)$

and μ_{nc} approaches $\mu(\omega)$. From the table, TA and ETD have leading truncation error of second-order, while TF and TB show first-order leading truncation error. These further ascertain the temporal accuracy discussed in the previous section.

3.5.1 Resolving Both Wavelength and Skin Depth

From Maxwell's equations, the analytical attenuation constant, α_0 and phase constant, β_0 in a doubly lossy medium can be solved as

$$\alpha_0 = \omega \left\{ \frac{\mu' \epsilon'}{2} \left[\sqrt{\left(1 - \frac{\mu'' \epsilon''}{\mu' \epsilon'}\right)^2 + \left(\frac{\mu''}{\mu'} + \frac{\epsilon''}{\epsilon'}\right)^2} - \left(1 - \frac{\mu'' \epsilon''}{\mu' \epsilon'}\right) \right] \right\}^{\frac{1}{2}} \quad (3.5.2a)$$

$$\beta_0 = \omega \left\{ \frac{\mu' \epsilon'}{2} \left[\sqrt{\left(1 - \frac{\mu'' \epsilon''}{\mu' \epsilon'}\right)^2 + \left(\frac{\mu''}{\mu'} + \frac{\epsilon''}{\epsilon'}\right)^2} + \left(1 - \frac{\mu'' \epsilon''}{\mu' \epsilon'}\right) \right] \right\}^{\frac{1}{2}} \quad (3.5.2b)$$

where $\epsilon' = \epsilon$, $\epsilon'' = \sigma/\omega$, $\mu' = \mu$ and $\mu'' = \sigma^*/\omega$. In electrically lossy media ($\sigma^* = 0$), $\mu'' = 0$ and (3.5.2) will recover the propagation constant derived in most electromagnetic textbooks, e.g. [109]. The medium wavelength and skin depth can then be found by $2\pi/\beta_0$ and $1/\alpha_0$, respectively. In most previous numerical studies of electrically lossy media, the cell size of a particular FDTD scheme is selected such that it sufficiently resolves the wavelength of the medium (usually at least 1/10 of wavelength for tolerable numerical errors) while disregarding the skin depth. This is permissible in electrically lossy media due to the fact that α_0 is always smaller than β_0 if $\mu'' = 0$. In fact, in highly lossy conductor ($\epsilon''/\epsilon' \gg 1$), $\alpha_0 \approx \beta_0$, and therefore, sufficiently resolved wavelength automatically guarantees sufficiently resolved skin depth. However in doubly lossy media, α_0 is not always smaller than β_0 for nonzero μ'' . A closer look at (3.5.2) reveals that when $\mu'' \epsilon''/\mu' \epsilon' > 1$, $\alpha_0 > \beta_0$. Under such circumstances, even if the wavelength is well resolved, the skin depth can be much smaller than the wavelength and still remains under-resolved which in turn yields higher numerical errors.

Figure 3.4: (a) Phase velocity and (b) attenuation errors with respect to $\sigma/\omega\epsilon$. $\sigma^*/\omega\mu = 10^{-2}$, CPW=40.

To further illustrate this, let us investigate the dispersion errors of FDTD schemes in doubly lossy media. We first assume 1-D propagation in z direction involving E_x and H_y field components. The only wavenumber k_z that exists can be solved explicitly from (3.5.1) as

$$k_z = \frac{2}{\Delta z} \arcsin \left(\frac{\Delta z \sqrt{\mu_{nc} \epsilon_{nc}}}{\Delta t} \sin \left(\frac{\omega \Delta t}{2} \right) \right) \quad (3.5.3)$$

The solution k_z will be complex in nature because of propagation in doubly lossy media. The numerical attenuation constant, phase constant and phase velocity can be found as $\alpha = -\text{Im}(k_z)$, $\beta = \text{Re}(k_z)$ and $v = \omega/\beta$ respectively. We further define two performance measures, which are the attenuation error, $(\alpha - \alpha_0)/\alpha_0$ and phase velocity error, $(v - v_0)/v_0$ where v_0 is the analytical phase velocity.

Fig. 3.4 plots the phase velocity and attenuation errors with respect to $\sigma/\omega\epsilon$ with $\sigma^*/\omega\mu = 10^{-2}$ and CPW equals 40. Δt is set at the 1-D lossless Courant limit $\Delta z \sqrt{\mu\epsilon}$ for ETD, TA, TF while for TB, smaller-than-lossless Courant limit is used due to the more stringent stability criterion. Note that the wavelength used is the

wavelength in doubly lossy media, given by $2\pi/\beta_0$ and should not be confused with the lossless media wavelength $2\pi/(\omega\sqrt{\mu\epsilon})$. We first note that TF and TB generally have higher magnitudes of phase and attenuation errors compared to ETD and TA at lower $\sigma/\omega\epsilon$. This is expected as TF and TB are only first-order accurate in time while ETD and TA are both second-order. More importantly, regardless of schemes, we observe that both phase velocity and attenuation errors increase dramatically beyond $\sigma/\omega\epsilon = 10^2$ because it is beyond this point that $\alpha_0 > \beta_0$ and the skin depth becomes under-resolved. This indicates the necessity to properly resolve skin depth for $\mu''\epsilon''/\mu'\epsilon' > 1$, which will be shown later.

3.5.2 3-D Dispersion Analysis

Since the dispersion errors become increasingly large for $\mu''\epsilon''/\mu'\epsilon' > 1$, the skin depth will be properly resolved in the 3-D analysis here. In the subsequent analysis, instead of specifying only CPW, uniform cell size Δ is chosen such that for positive integer N , Δ is λ/N if $\mu''\epsilon''/\mu'\epsilon' \leq 1$, and $2\pi\delta_s/N$ if $\mu''\epsilon''/\mu'\epsilon' > 1$, where λ is the medium wavelength and δ_s is the skin depth. Larger N implies higher mesh density. These criteria will ensure that the cell size always properly resolves both wavelength and skin depth. 2π is included because the ratio between wavelength and skin depth is exactly 2π at $\alpha_0 = \beta_0$. Alternatively, one may also specify Δ in terms of the magnitude of complex wavenumber. The magnitude of complex wavenumber, $|k_0|$ can be found from (3.5.2) as

$$|k_0| = \sqrt{\alpha_0^2 + \beta_0^2} = \omega \left\{ \mu'\epsilon' \sqrt{\left(1 - \frac{\mu''\epsilon''}{\mu'\epsilon'}\right)^2 + \left(\frac{\mu''}{\mu'} + \frac{\epsilon''}{\epsilon'}\right)^2} \right\}^{\frac{1}{2}} \quad (3.5.4)$$

However, specifying Δ in this may result in finer-than-necessary cell size, which increases computational effort undesirably, especially when $\alpha_0 = \beta_0$. Therefore, the former choice of specifying Δ in terms of λ or $2\pi\delta_s$ (depending on $\mu''\epsilon''/\mu'\epsilon'$)

Figure 3.5: Phase velocity error for (a) ETD, (b) TA, (c) TF and (d) TB with respect to θ and ϕ . $\sigma/\omega\epsilon = \sigma^*/\omega\mu = 10^2$, $N=10$.

is preferred over the latter in terms of $|k_0|$. In 3-D, there exist three individual wave vectors, $k_x = k \sin \theta \cos \phi$, $k_y = k \sin \theta \sin \phi$ and $k_z = k \cos \theta$ where θ is the longitudinal angle, ϕ is the azimuthal angle and $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$. The complex wavenumber k is then solved from (3.5.1) using appropriate root finding algorithm.

Fig. 3.5 shows the 3-D plot of phase velocity error for all schemes at different propagation angle in the first octant. $\sigma/\omega\epsilon = \sigma^*/\omega\mu = 10^2$, which gives $\mu''\epsilon''/\mu'\epsilon' = 10^4 > 1$, and N is selected as 10. Δt is now set at the 3-D lossless Courant limit $\Delta\sqrt{3\mu\epsilon}$ for

ETD, TA and TF while again for TB, it is set lower due to more stringent stability criterion. We see that, with properly resolved skin depth, the error level is not as high as in previous case. We also notice that second-order schemes ETD and TA have lower error magnitude than the first-order schemes TF and TB. On top of that, ETD has lower error compared to TA due to its closer resemblance to the solution of first-order differential equation. Furthermore, only TF has negative phase velocity error as opposed to others, which indicates that its phase velocity lags behind the analytical phase velocity while others lead. It will be shown later that for most of the values of $\sigma/\omega\epsilon$ and $\sigma^*/\omega\mu$, TF has opposing polarity of both phase velocity and attenuation errors compared to others. Since TB is only first-order accurate in time (higher error), and has more restrictive stability criterion compared to others, it shall be omitted in all our further comparisons. It should be reminded that unlike in 3-D lossless FDTD scheme where the numerical phase velocity always lags the analytical, it is generally not true in doubly lossy media. Also, the fact that lossless 3-D FDTD scheme always yields the lowest and highest phase velocity errors in the diagonal and axial directions does not generally apply for doubly lossy media.

In 3-D dispersion analysis, the more appropriate measures would be to find the maximum phase velocity and attenuation errors across all propagation angles (first octant will suffice as the dispersion error pattern repeats in every octant). We now define the positive maximum phase velocity error as $(\max[v(\theta, \phi)] - v_0)/v_0$ for $\max[v(\theta, \phi)] > v_0$, and the corresponding negative maximum phase velocity error as $(\min[v(\theta, \phi)] - v_0)/v_0$ for $\min[v(\theta, \phi)] < v_0$. Note that there is no positive maximum error if $v(\theta, \phi) < v_0$, and no negative maximum error if $v(\theta, \phi) > v_0$ for all angles. The positive and negative maximum attenuation errors are also defined in a similar fashion. Such definitions ensure that both “most positive” and “most negative” errors can be recorded.

Figure 3.6: Positive and negative maximum (a) phase velocity and (b) attenuation errors with respect to $\sigma/\omega\epsilon$. $\sigma^*/\omega\mu = 10^{-2}$, $N=40$. Dash lines represent negative maximum errors.

Figs. 3.6, 3.7 and 3.8 plot the positive and negative maximum phase velocity and attenuation errors with respect to $\sigma/\omega\epsilon$ at three cases of $\sigma^*/\omega\mu = 10^{-2}$, 10^0 and 10^2 . N is 40 and Δt is the 3-D lossless Courant limit throughout the remaining sections. Although not shown, it is found that the phase velocity and attenuation errors recorded for $\sigma^*/\omega\mu = 0$ and $\sigma^*/\omega\mu = 10^{-2}$ are very similar. Hence it can be understood that the dispersion characteristics of doubly lossy media at low $\sigma^*/\omega\mu$ ($< 10^{-2}$) do not differ much from that of electrically lossy media. It should also be noted that not all regions have simultaneous positive and negative maximum errors. Some may have either only positive or negative errors across all propagation angles. Next, we observe that in all cases, TF (first-order) generally displays higher (absolute) maximum errors than ETD and TA (second-order), and its maximum errors are mostly negative. Further comparing ETD and TA, it can be seen again that ETD generally has lower maximum errors than TA.

We note that the dispersion errors of TF can sometimes be lower than ETD and TA for certain $\sigma/\omega\epsilon$ and $\sigma^*/\omega\mu$ during the transition between negative maximum and

Figure 3.7: Same as Fig. 3.6, but for $\sigma^*/\omega\mu = 10^0$.

positive maximum errors (for instance, cf. Fig. 3.6). This effect is more pronounced in lower mesh density. To demonstrate this, Figs. 3.9 and 3.10 now plot the positive and negative maximum phase velocity and attenuation errors with respect to a range of frequencies at $N = 10$ and $N = 40$. Note that N is set with respect to the highest frequency (10 GHz), and Δ shall remain invariant for other lower frequencies. σ and σ^* are arbitrarily set at 60S/m and 800 Ω /m respectively. It can be seen that at $N = 10$ (low mesh density), the maximum phase velocity and attenuation errors exhibited by TF are lower than that of ETD and TA, and its maximum errors are in the same polarity as ETD and TA. At $N = 40$, the maximum errors of TF return to the highest among all. Such observations are somewhat similar to those found in [110], where higher order schemes do not necessarily yield lower dispersion errors at lower mesh density. Nevertheless, the dispersion errors of ETD are still lower than TA throughout.

Since the dispersion errors in 3-D differ at different angles, it is customary for us to define the phase velocity anisotropy error as $(\max[v(\theta, \phi)] - \min[v(\theta, \phi)]) / \min[v(\theta, \phi)]$. The attenuation anisotropy error is also defined in the similar way. Note that the

Figure 3.8: Same as Fig. 3.6, but for $\sigma^*/\omega\mu = 10^2$.

definition of anisotropy here is more appropriate compared to those in [93], where only diagonal and axial errors are taken in consideration. Figs. 3.11, 3.12 and 3.13 plot the phase velocity and attenuation anisotropy errors with respect to $\sigma/\omega\epsilon$ at $\sigma^*/\omega\mu = 10^{-2}$, 10^0 and 10^2 . N is set at 40. ETD and TA have near similar anisotropy errors while TF has generally higher anisotropy errors than ETD and TA. However, it can also be seen that the anisotropy errors of TF can be lower than that of ETD and TA at certain higher range of $\mu''\epsilon''/\mu'\epsilon'$. Again, similar to previous phase velocity and attenuation errors, this can be mitigated by adopting higher mesh density.

3.5.3 Numerical Simulation

In this subsection, further investigations with actual FDTD simulations in 1-D and 3-D are done. For 1-D, we use 100 cells of homogeneous doubly lossy medium with $\sigma = 10\text{S/m}$ and $\sigma^* = 10^4\Omega/\text{m}$. The values of σ and σ^* are chosen such that they are sufficiently large for clear demonstration of the doubly lossy effect, while ensuring measurable field values (not too severely attenuated). N is set at

Figure 3.9: Positive and negative maximum (a) phase velocity and (b) attenuation errors with respect to frequency. No negative maximum errors here. $\sigma = 60\text{S/m}$, $\sigma^* = 800\Omega/\text{m}$, $N = 10$ at $f_{max} = 10\text{GHz}$.

10 ($\Delta z = 10\mu\text{m}$) at the operating frequency of 100 GHz and $\Delta t = 0.811\text{ps}$ is at the lossless 1-D Courant limit. A Gaussian pulse with significant frequency content of up to 100 GHz is launched as a hard source at the initial point. The analytical electric field in time domain at each cell position after arbitrary time step can be obtained by numerically integrating the frequency domain solution. This analytical electric field will serve as the reference solution to be compared with the simulated electric field. Fig. 3.14a plots the absolute electric field error normalized to the maximum amplitude of reference solution against cell position. The error exhibited by TF has fallen outside the range of the plot and is comparatively larger than ETD and TA. Between second-order ETD and TA, we can see that the error recorded by ETD is generally lower than that of TA.

For 3-D experiment, we consider a homogeneous doubly lossy medium filled cavity with $18 \times 18 \times 17$ dimension terminated by PEC walls. σ and σ^* are chosen as 0.1S/m and $500\Omega/\text{m}$ respectively. A z -directed point current source is located precisely at the centre (10,10,9) of the cavity, driven by modulated Gaussian pulse with

Figure 3.10: Same as Fig. 3.9, but for $N = 40$. Dash lines represent negative maximum errors.

significant frequency content of up to 600 MHz. Again, $N = 10$ ($\Delta x = \Delta y = \Delta z = 36\text{mm}$) at the operating frequency of 600 MHz is chosen for the cell size, and $\Delta t = 69.267\text{ps}$ is at 3-D lossless Courant limit. The electric field is then recorded at position (16,16,15) until the simulation is terminated after 20ns. Using similar configuration, the cell size is reduced to 1/3 of the original problem and simulation is carried out using TA scheme with properly scaled dimension, cell size, and time step. This will serve as the reference solution for comparison. Fig. 3.14b plots the absolute electric field error normalized to the maximum amplitude of reference solution with respect to time. It can be seen that the error recorded by ETD is the lowest among all under such circumstances. Also, the overall errors recorded from 3-D experiment are larger than those recorded from 1-D. This may be due to the presence of anisotropy effects in 3-D. From all these simulations, we find that ETD is generally the better choice for modeling doubly lossy media compared to TA and TF.

Figure 3.11: (a) Phase velocity and (b) attenuation anisotropy errors with respect to $\sigma/\omega\epsilon$. $\sigma^*/\omega\mu = 10^{-2}$, $N = 40$.

3.6 Z-Transform and Corrected Impulse Invariance

The relationship between a continuous time input $x(t)$ and output $y(t)$ is often described in frequency domain as

$$\tilde{Y}(\omega) = \tilde{H}(\omega) \tilde{X}(\omega) \quad (3.6.1)$$

where $\tilde{H}(\omega)$ is the transfer function of the system in frequency domain. The Z-transform will find much usefulness for obtaining the discrete time samples of the output $y(t)$ if we can specify the relationship between the input and output in Z domain such that

$$\tilde{Y}(z) = \tilde{H}(z) \tilde{X}(z) \quad (3.6.2)$$

The question which remains is how to convert $\tilde{H}(\omega)$ into $\tilde{H}(z)$ accurately. To this end, by applying the frequency shifting property of the Fourier transform to the

Figure 3.12: Same as Fig. 3.11, but for $\sigma^*/\omega\mu = 10^0$.

Poisson summation formula, it can be shown that

$$\sum_{n=-\infty}^{\infty} h(n\Delta t) e^{-j\omega n} = \frac{1}{\Delta t} \sum_{k=-\infty}^{\infty} \tilde{H}\left(\frac{\omega - 2\pi k}{\Delta t}\right) \quad (3.6.3)$$

where $h(t)$ is the impulse response and Δt is the time step or sampling period. Equation (3.6.3) indicates that the sampling process of a continuous time signal will produce multiple copies of its own Fourier transform periodically. It can be further recognized that the left hand side of (3.6.3) is exactly the discrete time Fourier transform of the sampled impulse response $h[n]$ or more importantly, its Z-transform evaluated on the unit circle of Z plane. Thus, the relationship between the frequency and Z domains of a function is established and governed by (3.6.3).

In FDTD schemes for dispersive media, the analogy to the systems described in (3.6.1) and (3.6.2) are in two folds. Firstly, the electric and magnetic fields are related to their respective flux densities by frequency-dependent permittivity and permeability. Secondly, the FDTD operates in a discrete time scheme. In [37] and [38], the author made use of the classical impulse invariance method, which unfortunately, is inaccurate when the (causal) impulse response $h(t)$ of the media

Figure 3.13: Same as Fig. 3.11, but for $\sigma^*/\omega\mu = 10^2$.

is discontinuous at initial time $t = 0$ [111, 112]. The crux of the inaccuracy lies in the inappropriately chosen value of the discrete $h[0]$, where it is directly assumed from the initial value theorem as $h(0^+)$. The consequence is that the Z-transform of $h[n]$ violates (3.6.3) under such circumstances. To avoid this violation, correction is therefore needed for the original classical impulse invariance method.

For more clarity, consider a causal exponentially decaying impulse response $e^{-\alpha t}u(t)$ where $u(t)$ is the unit step function. Note that this exponentially decaying impulse response has discontinuity at $t = 0$ and the initial value theorem specifies that $h(0^+)$ equals one, which renders the classical impulse invariance method to choose $h[0]$ erroneously as unity. To find the correct value of $h[0]$ such that (3.6.3) is satisfied, we can further examine from (3.6.3) that $h[0]$ is nothing more than the Fourier series coefficient of $\sum_{k=-\infty}^{\infty} \frac{1}{\Delta t} \tilde{H}\left(\frac{\omega - 2\pi k}{\Delta t}\right)$ at $n = 0$. Recognizing that the Fourier transform of $e^{-\alpha t}u(t)$ is $\tilde{H}(\omega) = \frac{1}{j\omega + \alpha}$, we can write

$$h[0] = \frac{1}{2\pi} \int_0^{2\pi} \sum_{k=-\infty}^{\infty} \frac{1}{\Delta t} \frac{1}{\frac{j(\omega - 2\pi k)}{\Delta t} + \alpha} d\omega \quad (3.6.4)$$

Figure 3.14: Normalized absolute electric field error with respect to (a) cell position for 1-D problem and (b) time for 3-D problem in a doubly lossy medium. $N = 10$.

Upon some manipulations, we have

$$\frac{1}{2\pi} \int_0^{2\pi} \sum_{k=-\infty}^{\infty} \frac{1}{\Delta t} \frac{1}{j(\omega - 2\pi k) + \alpha} d\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{j\omega + \alpha\Delta t} d\omega \quad (3.6.5)$$

The value of $h[0]$ is finally determined as

$$h[0] = \lim_{\nu \rightarrow \infty} \frac{1}{\pi} \tan^{-1} \left(\frac{\nu}{\alpha\Delta t} \right) = \frac{1}{2} \quad (3.6.6)$$

Note that for convergence of (3.6.3), $\alpha > 0$ and $h[0]$ is only half the value as it was previously assumed using the classical impulse invariance method. This must be taken into consideration when Z-transform is performed on $h[n]$. Essentially, if the Z-transform is weighted with Δt (as in the classical impulse invariance method), subtraction of $\frac{\Delta t}{2}$ must be made to it.

For other forms of impulse response, a table of conversion among time, frequency and Z domains is provided, c.f. Table 3.5. The entries for classical impulse invariance method used in [37, 38] and corrected impulse invariance method are included together for direct comparison. It should be noted that the Z domain is weighted

Table 3.5: Conversion among time, frequency and Z domains. ©2009 IEEE.

Time Domain	Frequency Domain	Z Domain (classical impulse invariance)	Z Domain (corrected impulse invariance)
$\delta(t)$	1	1	1
$u(t)$	$\frac{1}{j\omega}$	$\frac{\Delta t}{1-z^{-1}}$	$\frac{\Delta t}{2} \left(\frac{1+z^{-1}}{1-z^{-1}} \right)$
$e^{-\alpha t} u(t)$	$\frac{1}{j\omega + \alpha}$	$\frac{\Delta t}{1-e^{-\alpha \Delta t} z^{-1}}$	$\frac{\Delta t}{2} \left(\frac{1+e^{-\alpha \Delta t} z^{-1}}{1-e^{-\alpha \Delta t} z^{-1}} \right)$
$\frac{\partial}{\partial t} \left(e^{-\alpha t} u(t) \right)$	$\frac{j\omega}{j\omega + \alpha}$	$1 - \frac{\alpha \Delta t}{1-e^{-\alpha \Delta t} z^{-1}}$	$1 - \frac{\alpha \Delta t}{2} \left(\frac{1+e^{-\alpha \Delta t} z^{-1}}{1-e^{-\alpha \Delta t} z^{-1}} \right)$
$e^{-\alpha t} \cos(\beta t) u(t)$	$\frac{\alpha + j\omega}{\alpha^2 + \beta^2 + 2\alpha j\omega - \omega^2}$	$\frac{\Delta t (1 - e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1})}{1 - 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} + e^{-2\alpha \Delta t} z^{-2}}$	$\frac{\Delta t (1 - e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1})}{1 - 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} + e^{-2\alpha \Delta t} z^{-2}} - \frac{\Delta t}{2}$
$e^{-\alpha t} \sin(\beta t) u(t)$	$\frac{\beta}{\alpha^2 + \beta^2 + 2\alpha j\omega - \omega^2}$	$\frac{\Delta t e^{-\alpha \Delta t} \sin(\beta \Delta t) z^{-1}}{1 - 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} + e^{-2\alpha \Delta t} z^{-2}}$	$\frac{\Delta t e^{-\alpha \Delta t} \sin(\beta \Delta t) z^{-1}}{1 - 2e^{-\alpha \Delta t} \cos(\beta \Delta t) z^{-1} + e^{-2\alpha \Delta t} z^{-2}}$

with the time step, Δt . For the time domain dirac delta function, no weighing of Δt is required on its frequency and Z domains. Both classical and corrected impulse invariance methods directly inherit unity from the frequency domain to preserve the linearity property of the Fourier and Z transforms. For all the other entries, their Z domains obtained using the corrected impulse invariance method have been properly corrected. The correction needed is the subtraction of $\frac{\Delta t}{2}$ to their original Z domain obtained using the classical impulse invariance method. Alternatively, the subtraction can also be viewed as inclusion of an additional zero with opposite polarity to the pole of the Z domain transfer function.

In fact, all the corrections tabulated in Table 3.5 can be further justified by reusing the exponentially decaying impulse response described earlier to find their respective $h[0]$. For unit time step $u(t)$, we can find its $h[0]$ by letting α in (3.6.4) to be vanishingly small. It follows from (3.6.6) that $h[0]$ is also half instead of unity assumed by the classical impulse invariance method. For the time derivative of exponentially decaying impulse response, we can rewrite the frequency domain transfer function as $\frac{j\omega}{j\omega + \alpha} = 1 - \frac{\alpha}{j\omega + \alpha}$ and obtain the Z domain transfer function readily. The last two entries belong to the second order pole transfer function. With the aid of complex

conjugate splitting, the value of $h[0]$ can still be determined conveniently. For the exponentially decaying cosine impulse response, it can be shown that

$$\begin{aligned} h[0] &= \lim_{\nu \rightarrow \infty} \left[\frac{1}{2\pi} \tan^{-1} \left(\frac{\nu}{p\Delta t} \right) + \frac{1}{2\pi} \tan^{-1} \left(\frac{\nu}{p^*\Delta t} \right) \right] \\ &= \frac{1}{2} \end{aligned} \quad (3.6.7)$$

where $p = \alpha + j\beta$. Again, $h[0]$ is only half as opposed to unity assumed by the classical impulse invariance method. Finally, for the exponentially decaying sine impulse response, its value of $h[0]$ can be shown as

$$\begin{aligned} h[0] &= \lim_{\nu \rightarrow \infty} \left[\frac{j}{2\pi} \tan^{-1} \left(\frac{\nu}{p\Delta t} \right) - \frac{j}{2\pi} \tan^{-1} \left(\frac{\nu}{p^*\Delta t} \right) \right] \\ &= 0 \end{aligned} \quad (3.6.8)$$

In this case, $h[0]$ is found to be zero. Therefore, the impulse response is not discontinuous at $t = 0$, and no further subtraction of $\frac{\Delta t}{2}$ is needed for its Z domain transfer function obtained using the classical impulse invariance method.

Notably, the (first-order) exponentially decaying impulse response represents the form of time domain susceptibility function of a Debye medium. In the following, we will present various formulations for Debye media using the corrected impulse invariance method.

3.7 Formulations for Debye Dispersive Media

For a Debye medium having multiple first order poles, the complex relative permittivity is characterized by

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p}{1 + j\omega\tau_p} \quad (3.7.1)$$

It should be noted that the time domain impulse response of (3.7.1) is discontinuous at $t = 0$. In the following subsections, the formulations from three different relations using both corrected and classical impulse invariance methods will be shown, along with their respective memory storage requirements. With the help of Table 3.5, the conversion from frequency to Z domain can be done conveniently. The update equations in time domain can then be easily obtained from the Z domain equations by recognizing that the z^{-1} operator denotes the value at one time step earlier.

3.7.1 Formulation from D and E Relation

The dependency between two phasors $\tilde{\mathbf{D}}$ and $\tilde{\mathbf{E}}$ is given by

$$\tilde{\mathbf{D}}(\omega) = \left(\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \Delta \epsilon_p}{1 + j\omega \tau_p} + \frac{\sigma}{j\omega} \right) \tilde{\mathbf{E}}(\omega) \quad (3.7.2)$$

where the conductivity, σ has also been included.

We now invoke the corrected impulse invariance to (3.7.2) to obtain the Z domain equation as

$$\tilde{\mathbf{D}}(z) = \left(\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \Delta \epsilon_p \Delta t / \tau_p}{1 - e^{-\Delta t / \tau_p} z^{-1}} + \frac{\sigma \Delta t}{2} \left(\frac{1 + z^{-1}}{1 - z^{-1}} \right) \right) \tilde{\mathbf{E}}(z) \quad (3.7.3)$$

Introducing the intermediate variables $\tilde{\mathbf{S}}_p(z)$, $\tilde{\mathbf{I}}(z)$,

$$\tilde{\mathbf{S}}_p(z) = \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} \left(\frac{e^{-\Delta t / \tau_p}}{1 - e^{-\Delta t / \tau_p} z^{-1}} \right) \tilde{\mathbf{E}}(z) \quad (3.7.4a)$$

$$\tilde{\mathbf{I}}(z) = \left(\frac{\sigma \Delta t}{1 - z^{-1}} \right) \tilde{\mathbf{E}}(z) \quad (3.7.4b)$$

and upon some manipulations, the set of time domain update equations read:

$$\mathbf{D}^{n+1} = \mathbf{D}^n + \Delta t \nabla \times \mathbf{H}^{n+\frac{1}{2}} \quad (3.7.5a)$$

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} - \sum_p \mathbf{S}_p^n - \mathbf{I}^n}{\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{2\tau_p} + \frac{\sigma \Delta t}{2}} \quad (3.7.5b)$$

$$\mathbf{S}_p^{n+1} = \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} e^{-\frac{\Delta t}{\tau_p}} \mathbf{E}^{n+1} + e^{-\frac{\Delta t}{\tau_p}} \mathbf{S}_p^n \quad (3.7.5c)$$

$$\mathbf{I}^{n+1} = \sigma \Delta t \mathbf{E}^{n+1} + \mathbf{I}^n \quad (3.7.5d)$$

The H fields are still updated as in the Yee's explicit FDTD method throughout.

For comparison, invoking only the classical impulse invariance method to (3.7.2) will replace (3.7.5b) by

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} - \sum_p \mathbf{S}_p^n - \mathbf{I}^n}{\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \Delta \epsilon_p \Delta t}{\tau_p} + \sigma \Delta t} \quad (3.7.6)$$

with the rest of (3.7.5) remain unchanged. Hereby, we point out that the difference posed by the corrected version compared to the classical impulse invariance method lies in the denominator terms of (3.7.6). For these two methods that originate from the relation between D and E , we shall refer to the corrected impulse invariance method as DE_{cor} and its classical impulse invariance method counterpart only as DE .

3.7.2 Formulation from $\mathbf{P}$ and $\mathbf{E}$ Relation

The formulation in this subsection makes use of another relation described by

$$\tilde{\mathbf{P}}_p(\omega) = \frac{\epsilon_0 \Delta \epsilon_p}{1 + j\omega \tau_p} \tilde{\mathbf{E}}(\omega) \quad (3.7.7)$$

where $\mathbf{P}$ (without tilde in time domain) is associated to Ampere's law as

$$\nabla \times \mathbf{H} = \epsilon_0 \epsilon_\infty \frac{\partial}{\partial t} \mathbf{E} + \sigma \mathbf{E} + \sum_p \frac{\partial}{\partial t} \mathbf{P}_p \quad (3.7.8)$$

Invoking corrected impulse invariance method to (3.7.7), we obtain the Z domain equation as

$$\tilde{\mathbf{P}}_p(z) = \left(\frac{\epsilon_0 \Delta \epsilon_p \Delta t}{2\tau_p} \left(\frac{1 + e^{-\Delta t/\tau_p}}{1 - e^{-\Delta t/\tau_p}} \right) \right) \tilde{\mathbf{E}}_p(z). \quad (3.7.9)$$

Further combination with central difference approximation and time averaging of Ampere's law in (3.7.8), one gets the final update equations as

$$\mathbf{E}^{n+1} = c_1^{PE} \mathbf{E}^n + c_2^{PE} \left(\nabla \times \mathbf{H}^{n+\frac{1}{2}} - \frac{1}{\Delta t} \sum_p (k_{1p}^{PE} - 1) \mathbf{P}^n \right) \quad (3.7.10a)$$

$$\mathbf{P}_p^{n+1} = k_{1p}^{PE} \mathbf{P}_p^n + k_{2p}^{PE} \mathbf{E}^{n+1} + k_{3p}^{PE} \mathbf{E}^n \quad (3.7.10b)$$

where

$$c_1^{PE} = \left(\frac{2\epsilon_0\epsilon_\infty - 2\sum_p k_{3p}^{PE} - \sigma\Delta t}{2\epsilon_0\epsilon_\infty + 2\sum_p k_{2p}^{PE} + \sigma\Delta t} \right)$$

$$c_2^{PE} = \left(\frac{2\Delta t}{2\epsilon_0\epsilon_\infty + 2\sum_p k_{2p}^{PE} + \sigma\Delta t} \right)$$

$$k_{1p}^{PE} = e^{-\frac{\Delta t}{\tau_p}}$$

$$k_{2p}^{PE} = \epsilon_0\Delta\epsilon_p\Delta t/2\tau_p$$

$$k_{3p}^{PE} = k_{1p}^{PE} k_{2p}^{PE}$$

On the other hand, the final update equations resulting from classical impulse invariance method have the same form as (3.7.10a)-(3.7.10b), but with the following update coefficients replaced

$$k_{2p}^{PE} = \epsilon_0\Delta\epsilon_p\Delta t/\tau_p$$

$$k_{3p}^{PE} = 0$$

For these two methods that originate from the relation between P and E , we shall refer to the corrected impulse invariance method as PE_{cor} and its classical impulse invariance method counterpart only as PE .

3.7.3 Formulation from $\mathbf{J}$ and $\mathbf{E}$ Relation

Alternatively, there exists another relation of the form

$$\tilde{\mathbf{J}}_p(\omega) = \frac{j\omega\epsilon_0\Delta\epsilon_p}{1 + j\omega\tau_p} \tilde{\mathbf{E}}(\omega) \quad (3.7.11)$$

where $\mathbf{J}$ is associated to Ampere's law as

$$\nabla \times \mathbf{H} = \epsilon_0\epsilon_\infty \frac{\partial}{\partial t} \mathbf{E} + \sigma \mathbf{E} + \sum_p \mathbf{J}_p \quad (3.7.12)$$

Similarly, we invoke corrected impulse invariance method to (3.7.11) to obtain Z domain equation as

$$\tilde{\mathbf{J}}_p(z) = \frac{\epsilon_0\Delta\epsilon_p}{\tau_p} \left[\frac{\left(1 - e^{-\Delta t/\tau_p} z^{-1}\right) - \frac{\Delta t}{2\tau_p} \left(1 + e^{-\Delta t/\tau_p} z^{-1}\right)}{1 - e^{-\Delta t/\tau_p} z^{-1}} \right] \tilde{\mathbf{E}}(z) \quad (3.7.13)$$

Further combination with central difference approximation and time averaging of Ampere's law in(3.7.12), one gets the final update equations as

$$\mathbf{E}^{n+1} = c_1^{JE} \mathbf{E}^n + c_2^{JE} \left(\nabla \times \mathbf{H}^{n+\frac{1}{2}} - \frac{1}{2} \sum_p \left(k_{1p}^{JE} + 1 \right) \mathbf{J}_p^n \right) \quad (3.7.14a)$$

$$\mathbf{J}_p^{n+1} = k_{1p}^{JE} \mathbf{J}_p^n + k_{2p}^{JE} \mathbf{E}^{n+1} + k_{3p}^{JE} \mathbf{E}^n \quad (3.7.14b)$$

where

$$\begin{aligned} c_1^{JE} &= \left(\frac{2\epsilon_0\epsilon_\infty - \Delta t \sum_p k_{3p}^{JE} - \sigma \Delta t}{2\epsilon_0\epsilon_\infty + \Delta t \sum_p k_{2p}^{JE} + \sigma \Delta t} \right) \\ c_2^{JE} &= \left(\frac{2\Delta t}{2\epsilon_0\epsilon_\infty + \Delta t \sum_p k_{2p}^{JE} + \sigma \Delta t} \right) \\ k_{1p}^{JE} &= e^{-\frac{\Delta t}{\tau_p}} \\ k_{2p}^{JE} &= \frac{\epsilon_0\Delta\epsilon_p}{\tau_p} \left(1 - \frac{\Delta t}{2\tau_p} \right) \\ k_{3p}^{JE} &= -k_{1p}^{JE} \frac{\epsilon_0\Delta\epsilon_p}{\tau_p} \left(1 + \frac{\Delta t}{2\tau_p} \right) \end{aligned}$$

The formulated final update equations from classical impulse invariance method will

differ from (3.7.14a)-(3.7.14b) in terms of update coefficients given as

$$k_{2p}^{JE} = \frac{\epsilon_0 \Delta \epsilon_p}{\tau_p} \left(1 - \frac{\Delta t}{\tau_p} \right)$$

$$k_{3p}^{JE} = -k_{1p}^{JE} \frac{\epsilon_0 \Delta \epsilon_p}{\tau_p}$$

For these two methods that originate from the relation between J and E , we shall refer to the corrected impulse invariance method as JE_{cor} and its classical impulse invariance method counterpart only as JE .

3.7.4 Memory Storage Requirements

The memory storage requirements of FDTD methods for dispersive media is larger than that of a standard Yee's FDTD method for nondispersive media due to the need for additional auxiliary variables apart from E and H main field components. Table 3.6 shows the amount of memory storage per cell needed in Debye media. N_e and N_h are the number of electric and magnetic field components respectively, and N_p is the number of dispersion term used to model a particular dispersive medium. N_e and N_h are dictated by the problem dimension and N_p is specified as to how well a Debye model fits a particular medium's frequency-dependent permittivity (based on nonlinear least square analysis [114]). The entries for ADE [35] and PLRC [27] methods are also included for comparison.

From Table 3.6, it is clear that DE_{cor} and DE require larger memory storage than the others because their formulations involve more variables. By simply redefining the auxilliary variables, we can achieve lower memory requirements. In particular, PE_{cor} and JE_{cor} are of great interest because they represent the corrected versions of all the Z-transform schemes and they still retain the storage requirements as in the case of ADE and PLRC methods. For large 3-D problems, such savings in memory usage compared to DE_{cor} and DE are often desirable.

Table 3.6: Memory storage requirements for Debye media. ©2009 IEEE.

Method	Memory per Cell
DE_{cor}, DE	$2 N_e + N_h + N_e N_p$
$PE_{cor}, PE,$ $JE_{cor}, JE,$ $ADE, PLRC$	$N_e + N_h + N_e N_p$

3.8 Formulations For Lorentz Dispersive Media

For a Lorentz medium with multiple second-order poles, the complex relative permittivity is characterized by

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p \omega_p^2}{\omega_p^2 + 2j\omega\delta_p - \omega^2} \quad (3.8.1)$$

Similarly, the update equations can also be formulated from three different relations. After the conversion from frequency to Z domain via Table 3.5, the update equations in time domain are easily obtained from the Z domain equations by recognizing that the z^{-1} and z^{-2} operators denote the value at one and two time steps earlier.

3.8.1 Formulation from D and E Relation

The dependency between two phasors $\tilde{\mathbf{D}}$ and $\tilde{\mathbf{E}}$ is given by

$$\tilde{\mathbf{D}}(\omega) = \left(\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \beta_p \gamma_p}{\alpha_p^2 + \beta_p^2 + 2j\omega\alpha_p - \omega^2} + \frac{\sigma}{j\omega} \right) \tilde{\mathbf{E}}(\omega) \quad (3.8.2)$$

where for notational convenience, we define $\alpha_p = \delta_p$, $\beta_p = \sqrt{\omega_p^2 - \delta_p^2}$ and $\gamma_p = \Delta\epsilon_p \omega_p^2 / \beta_p$. It is pointed out here that the time domain susceptibility function of a Lorentz medium is not discontinuous at initial time zero due to its second order

pole which involves sine term. Therefore there is no correction needed for it. However, correction is still needed in the conductivity term. Invoking corrected impulse invariance method to (3.8.2) will result in the following:

$$\tilde{\mathbf{D}}(z) = \left(\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \Delta t \gamma_p e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t) z^{-1}}{1 - 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) z^{-1} + e^{-2\alpha_p \Delta t} z^{-2}} + \frac{\sigma \Delta t}{2} \left(\frac{1 + z^{-1}}{1 - z^{-1}} \right) \right) \tilde{\mathbf{E}}(z) \quad (3.8.3)$$

We also introduce two intermediate parameters, $\tilde{\mathbf{S}}_p(z)$ and $\tilde{\mathbf{I}}(z)$ as

$$\tilde{\mathbf{S}}_p(z) = \left(\frac{\Delta t \epsilon_0 \gamma_p e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t)}{1 - 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) z^{-1} + e^{-2\alpha_p \Delta t} z^{-2}} \right) \tilde{\mathbf{E}}(z) \quad (3.8.4a)$$

$$\tilde{\mathbf{I}}(z) = \left(\frac{\sigma \Delta t}{1 - z^{-1}} \right) \tilde{\mathbf{E}}(z) \quad (3.8.4b)$$

and upon some manipulations and collecting like terms, the final update equations read:

$$\mathbf{D}^{n+1} = \mathbf{D}^n + \nabla \times \mathbf{H}^{n+\frac{1}{2}} \quad (3.8.5a)$$

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} - \sum_p \mathbf{S}_p^n - \mathbf{I}^n}{\epsilon_0 \epsilon_\infty + \sigma \Delta t / 2} \quad (3.8.5b)$$

$$\mathbf{S}_p^{n+1} = 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) \mathbf{S}_p^n - e^{-2\alpha_p \Delta t} \mathbf{S}_p^{n-1} + \Delta t \epsilon_0 \gamma_p e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t) \mathbf{E}^{n+1}, \quad \forall p \quad (3.8.5c)$$

$$\mathbf{I}^{n+1} = \mathbf{I}^n + \sigma \Delta t \mathbf{E}^{n+1} \quad (3.8.5d)$$

For comparison, invoking only the classical impulse invariance method to (3.8.2) will replace (3.8.5b) with

$$\mathbf{E}^{n+1} = \frac{\mathbf{D}^{n+1} - \sum_p \mathbf{S}_p^n - \mathbf{I}^n}{\epsilon_0 \epsilon_\infty + \sigma \Delta t} \quad (3.8.6)$$

and it shall be noted that the only slight difference posed by the corrected impulse invariance method as compared to its classical impulse invariance method counterpart lies in the conductivity term. Hence, the classical impulse invariance method will not suffer from any inaccuracy whenever the conductivity of the medium is

zero. Similarly, the corrected impulse invariance method and its classical impulse invariance method counterpart here are referred to as DE_{cor} and DE respectively.

3.8.2 Formulation from $\mathbf{P}$ and $\mathbf{E}$ Relation

Alternatively, we can derive the update equations from another relation described by

$$\tilde{\mathbf{P}}_p(\omega) = \sum_p \frac{\epsilon_0 \beta_p \gamma_p}{\alpha_p^2 + \beta_p^2 + 2j\omega\alpha_p - \omega^2} \tilde{\mathbf{E}}(\omega) \quad (3.8.7)$$

where $\mathbf{P}$ is again associated to Ampere's law in (3.7.8).

Invoking corrected impulse invariance method to (3.8.7), we obtain the Z domain equations of

$$\tilde{\mathbf{P}}_p(z) = \sum_p \frac{\epsilon_0 \Delta t \gamma_p e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t) z^{-1}}{1 - 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) z^{-1} + e^{-2\alpha_p \Delta t} z^{-2}} \tilde{\mathbf{E}}(z). \quad (3.8.8)$$

Further combination with central difference approximation and time averaging of Ampere's law in (3.7.8), the final update equations read:

$$\mathbf{E}^{n+1} = c_1^{PE} \mathbf{E}^n + c_2^{PE} \left(\nabla \times \mathbf{H}^{n+\frac{1}{2}} - \frac{1}{\Delta t} \sum_p \left((k_{1p}^{PE} - 1) \mathbf{P}_p^n - k_{2p}^{PE} \mathbf{P}_p^{n-1} \right) \right) \quad (3.8.9a)$$

$$\mathbf{P}_p^{n+1} = k_{1p}^{PE} \mathbf{P}_p^n - k_{2p}^{PE} \mathbf{P}_p^{n-1} + k_{3p}^{PE} \mathbf{E}^n \quad (3.8.9b)$$

where

$$c_1^{PE} = \frac{2\epsilon_0\epsilon_\infty - \sigma\Delta t - 2\sum_p k_{3p}^{PE}}{2\epsilon_0\epsilon_\infty + \sigma\Delta t}$$

$$c_2^{PE} = \left(\frac{2\Delta t}{2\epsilon_0\epsilon_\infty + \sigma\Delta t} \right)$$

$$k_{1p}^{PE} = 2e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t)$$

$$k_{2p}^{PE} = e^{-2\alpha_p \Delta t}$$

$$k_{3p}^{PE} = \epsilon_0 \gamma_p \Delta t e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t).$$

It shall be pointed out specially that in this case, the classical impulse invariance method is exactly the same as the corrected impulse invariance method. This is because there is no correction needed in the first place as the time domain impulse response of (3.7.7) is continuous at initial time zero. Similarly, we shall refer to the corrected impulse invariance method as PE_{cor} and its classical impulse invariance method counterpart as PE .

3.8.3 Formulation for J and E Relation

Another relation that can be considered is given as

$$\tilde{\mathbf{J}}_p(\omega) = \sum_p \frac{j\omega\epsilon_0\beta_p\gamma_p}{\alpha_p^2 + \beta_p^2 + 2j\omega\alpha_p - \omega^2} \tilde{\mathbf{E}}_p(\omega) \quad (3.8.10)$$

where $\mathbf{J}$ is associated to Ampere's law in (3.7.12).

Invoking corrected impulse invariance method to (3.8.10), we obtain the Z domain equations of

$$\tilde{\mathbf{J}}_p(z) = \left(\frac{\Delta t\epsilon_0\beta_p\gamma_p/2 - \Delta t\epsilon_0\alpha_p\gamma_p e^{-\alpha_p\Delta t} \sin(\beta_p\Delta t)z^{-1} - \frac{\Delta t\epsilon_0\beta_p\gamma_p}{2} e^{-2\alpha_p\Delta t} z^{-2}}{1 - 2e^{-\alpha_p\Delta t} \cos(\beta_p\Delta t)z^{-1} + e^{-2\alpha_p\Delta t} z^{-2}} \right) \tilde{\mathbf{E}}(z). \quad (3.8.11)$$

Further combination with central difference approximation and time averaging of Ampere's law in (3.7.12), the final update equations read:

$$\mathbf{E}^{n+1} = c_1^{JE} \mathbf{E}^n + c_2^{JE} \mathbf{E}^{n-1} + c_3^{JE} \left(\nabla \times \mathbf{H}^{n+\frac{1}{2}} - \frac{1}{2} \sum_p \left((k_{1p}^{JE} + 1) \mathbf{J}_p^n - k_{2p}^{JE} \mathbf{J}_p^{n-1} \right) \right) \quad (3.8.12a)$$

$$\mathbf{J}_p^{n+1} = k_{1p}^{JE} \mathbf{J}_p^n - k_{2p}^{JE} \mathbf{J}_p^{n-1} + k_{3p}^{JE} \mathbf{E}^{n+1} - k_{4p}^{JE} \mathbf{E}^n - k_{5p}^{JE} \mathbf{E}^{n-1} \quad (3.8.12b)$$

where

$$c_1^{JE} = \frac{2\epsilon_0\epsilon_\infty - \sigma\Delta t + \Delta t \sum_p k_{4p}^{JE}}{2\epsilon_0\epsilon_\infty + \sigma\Delta t + \Delta t \sum_p k_{3p}^{JE}}$$

$$\begin{aligned}
c_2^{JE} &= \frac{\Delta t \sum_p k_{5p}}{2\epsilon_0\epsilon_\infty + \sigma\Delta t + \Delta t \sum_p k_{3p}^{JE}} \\
c_3^{JE} &= \frac{\Delta t}{2\epsilon_0\epsilon_\infty + \sigma\Delta t + \Delta t \sum_p k_{3p}^{JE}} \\
k_{1p}^{JE} &= 2e^{-\alpha_p\Delta t} \cos(\beta_p\Delta t) \\
k_{2p}^{JE} &= e^{-2\alpha_p\Delta t} \\
k_{3p}^{JE} &= \epsilon_0\Delta t\beta_p\gamma_p/2 \\
k_{4p}^{JE} &= \epsilon_0\alpha_p\gamma_p\Delta te^{-\alpha_p\Delta t} \sin(\beta_p\Delta t) \\
k_{5p}^{JE} &= k_{2p}k_{3p}
\end{aligned}$$

The formulated final update equations from classical impulse invariance method will differ from (3.8.12a)-(3.8.12b) in terms of update coefficients given as

$$\begin{aligned}
c_2 &= 0 \\
c_3^{JE} &= \frac{2\Delta t}{2\epsilon_0\epsilon_\infty + \sigma\Delta t + \Delta t \sum_p k_{3p}^{JE}} \\
k_{3p}^{JE} &= \epsilon_0\Delta t\beta_p\gamma_p \\
k_{4p}^{JE} &= \epsilon_0\gamma_p\Delta te^{-\alpha_p\Delta t} \left(\alpha_p \sin(\beta_p\Delta t) + \beta_p \cos(\beta_p\Delta t) \right) \\
k_{5p}^{JE} &= 0
\end{aligned}$$

Again, we refer the corrected impulse invariance method as JE_{cor} and its classical impulse invariance method counterpart as JE .

3.8.4 Memory Storage Requirements

From Table 3.7, the memory storage requirements for Lorentz media are generally larger than that for Debye media due to higher order poles, and thus the need for more back storages. PE_{cor} , PE , JE and PLRC present the lowest memory storage among all, where no more than one array is needed for the E fields. With the same amount of memory storage, PE_{cor} is simpler to use without the need for complex

Table 3.7: Memory storage requirements for Lorentz media

Method	Memory per Cell
$DE_{cor}, DE,$ $JE_{cor}, ADE,$	$2N_e + N_h + 2N_e N_p$
$PE_{cor}, PE,$ $JE, PLRC,$	$N_e + N_h + 2N_e N_p$

recursive accumulator as in PLRC method for Lorentz media. For ADE method, an alternative reformulation of the auxiliary variable [36] can be done to reduce the memory storage requirements to those in PE_{cor} , PE , JE and PLRC method.

3.9 Dispersion Relation and Complex Numerical Permittivity

Using Fourier analysis in conjunction with central difference on Yee's cell, the FDTD update equations for dispersive media can be represented as

$$-j\mathbf{K} \times \mathbf{H}_0 = j\Omega\epsilon_{nc}\mathbf{E}_0 \quad (3.9.1a)$$

$$j\mathbf{K} \times \mathbf{E}_0 = j\Omega\mu_{nc}\mathbf{H}_0 \quad (3.9.1b)$$

where

$$\Omega = 2 \sin(\omega\Delta t/2) / \Delta t$$

$$\mathbf{K} = K_x\hat{x} + K_y\hat{y} + K_z\hat{z}$$

$$K_\xi = 2 \sin(k_\xi\Delta\xi/2) / \Delta\xi$$

ϵ_{nc} and μ_{nc} are the complex numerical permittivity and permeability. For Yee's FDTD compatible methods, the update equations can be conveniently described

in the form of (3.9.1a)-(3.9.1b), with ϵ_{nc} and μ_{nc} varying according to the type of material and the particular modeling method. From (3.9.1a)-(3.9.1b), we are also able to see that $\mathbf{K} \cdot \mathbf{E}_0 = 0$ and $\mathbf{K} \cdot \mathbf{H}_0 = 0$, which are indications of Yee's FDTD divergence-free nature [2]. The dispersion relation can then be derived from (3.9.1a)-(3.9.1b) as

$$\mathbf{K} \cdot \mathbf{K} = \Omega^2 \mu_{nc} \epsilon_{nc} \quad (3.9.2)$$

For nondispersive, lossless media, ϵ_{nc} and μ_{nc} are constant values and (3.9.2) is reduced to dispersion relation of standard Yee's FDTD scheme. Since we only consider nonmagnetic materials here, μ_{nc} is assumed to be permeability of free space μ_0 . Extension into dispersive magnetic materials is also possible and very straight forward. It can be seen that (3.9.2) describes the dispersion relation of a particular FDTD method for dispersive media which is inherent from the complex numerical permittivity. Table 3.8 shows the list of complex numerical permittivity ϵ_{nc} of various Z-transform methods for Debye media. The leading error term of the complex numerical permittivity is the error term with the lowest order of Δt , obtained by performing Taylor series expansion of ϵ_{nc} and comparing to the analytical $\epsilon(\omega)$. Also shown in the table are the entries of ADE and PLRC methods for comparison. For other variations of direct integration and recursive convolution methods, readers can refer to [45].

Looking at Table 3.8, it is observed that all corrected impulse invariance methods for Debye media have leading error terms of one order higher than all classical impulse invariance methods with respect to Δt . This implies that corrected impulse invariance method indeed has temporal accuracy of one order higher than classical impulse invariance method. The order of temporal accuracy is also the same as both ADE and PLRC methods. It is also interesting to note that the complex

numerical permittivities of DE_{cor} and PE_{cor} are exactly the same although their update equations originate from different relations. Hence, PE_{cor} is an alternative reformulation of DE_{cor} which will yield the same computations but with less memory. For JE_{cor} , the transformation from frequency to Z domain is performed with an additional zero ($j\omega$) as seen from (3.7.11), which results in a different complex numerical permittivity than DE_{cor} and PE_{cor} .

Table 3.8: List of complex numerical permittivity and leading error term for Debye media. ©2009 IEEE.

Method	Complex Numerical Permittivity	Leading Error Term
DE_{cor}	$\epsilon_0\epsilon_\infty + \sum_p \frac{\epsilon_0\Delta\epsilon_p\Delta t}{2\tau_p} \coth(a) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2 \left(\sum_p \frac{\epsilon_0\Delta\epsilon_p}{12\tau_p^2} (1 + j\omega\tau_p) + \frac{j\omega\sigma}{12} \right)$
PE_{cor}	$\epsilon_0\epsilon_\infty + \sum_p \frac{\epsilon_0\Delta\epsilon_p\Delta t}{2\tau_p} \coth(a) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2 \left(\sum_p \frac{\epsilon_0\Delta\epsilon_p}{12\tau_p^2} (1 + j\omega\tau_p) + \frac{j\omega\sigma}{12} \right)$
JE_{cor}	$\epsilon_0\epsilon_\infty + \sum_p \frac{\Lambda\epsilon_0\Delta\epsilon_p}{j\Omega\tau_p} \left(1 - \frac{\Delta t}{2\tau_p} \coth(a) \right) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2 \left(\sum_p \frac{\epsilon_0\Delta\epsilon_p}{12\tau_p^2} \frac{(j-2\omega\tau_p-j\omega^2\tau_p^2-\omega^3\tau_p^3)}{\omega(1+j\omega\tau_p)} + \frac{j\omega\sigma}{12} \right)$
DE	$\epsilon_0\epsilon_\infty + \sum_p \frac{\epsilon_0\Delta\epsilon_p\Delta t}{2\tau_p} \frac{e^a}{\sinh(a)} + \frac{\sigma e^{j\omega\Delta t/2}}{j\Omega}$	$\Delta t \left(\sum_p \frac{\epsilon_0\Delta\epsilon_p}{2\tau_p} + \frac{\sigma}{2} \right)$
PE	$\epsilon_0\epsilon_\infty + \sum_p \frac{\epsilon_0\Delta\epsilon_p\Delta t}{2\tau_p} \frac{e^a}{\sinh(a)} + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t \sum_p \frac{\epsilon_0\Delta\epsilon_p}{2\tau_p}$
JE	$\epsilon_0\epsilon_\infty + \sum_p \frac{\Lambda\epsilon_0\Delta\epsilon_p}{j\Omega\tau_p} \left(1 - \frac{\Delta t}{2\tau_p} \frac{e^a}{\sinh(a)} \right) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t \sum_p \frac{j\epsilon_0\Delta\epsilon_p}{2\omega\tau_p^2}$
ADE	$\epsilon_0\epsilon_\infty + \sum_p \frac{\Lambda\epsilon_0\Delta\epsilon_p}{\Lambda+j\Omega\tau_p} + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2 \left(\sum_p \frac{-j\epsilon_0\Delta\epsilon_p\omega^3\tau_p}{12(1+j\omega\tau_p)^2} + \frac{j\omega\sigma}{12} \right)$
$PLRC$ (notations can be found in [27, 91])	$\epsilon_0\epsilon_\infty + \sum_p \frac{\lambda_p^0\epsilon_0 e^{j\omega\Delta t/2}}{j\Omega\Delta t} - \sum_p \epsilon_0\iota_p\lambda_p^0$ $- \sum_p \frac{\Delta\chi_p^0\epsilon_0 e^{\frac{\Delta t}{2\tau_p}} \left(1 + \iota_p (e^{-j\omega\Delta t} - 1) \right)}{j2\Omega\Delta t \sinh(a)} + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2 \left(\sum_p \frac{-\epsilon_0\Delta\epsilon_p\omega^2}{12(1+j\omega\tau_p)} + \frac{j\omega\sigma}{12} \right)$

$$a = \frac{\Delta t}{2\tau_p} + \frac{j\omega\Delta t}{2}, \quad \Lambda = \cos(\omega\Delta t/2)$$

For Lorentz media in Table 3.9, the corrected impulse invariance methods also have the same order of accuracy as ADE and PLRC method. They are of one order higher than the classical impulse invariance methods with respect to Δt , except for the case of PE because no correction is needed for the formulation of PE . For DE , although

having lower order of accuracy, the leading error term contains only the conductivity term. For JE , the leading error term involves parameters from the susceptibility function. Note also that the complex numerical permittivity of DE_{cor} is exactly the same as PE_{cor} although their update equations originate from different relations. For lorentz media, PE_{cor} is also an alternative reformulation of DE_{cor} which will yield the same computations but with less memory storage requirements.

Table 3.9: List of complex numerical permittivity and leading error term for Lorentz media

Method	Complex Numerical Permittivity	Leading Error Term
DE_{cor}	$\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \gamma \Delta t e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t)}{b} + \frac{\sigma \Lambda}{j \Omega}$	$\Delta t^2 \left(\sum_p \frac{-\epsilon_0 \beta_p \gamma_p}{12} + \frac{j \omega \sigma}{12} \right)$
PE_{cor}	$\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \gamma \Delta t e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t)}{b} + \frac{\sigma \Lambda}{j \Omega}$	$\Delta t^2 \left(\sum_p \frac{-\epsilon_0 \beta_p \gamma_p}{12} + \frac{j \omega \sigma}{12} \right)$
JE_{cor}	$\epsilon_0 \epsilon_\infty + \sum_p \frac{\Lambda \epsilon_0 \beta_p \gamma_p \frac{\Delta t}{2} (e^{j \omega \Delta t} - e^{-2 \alpha_p \Delta t - j \omega \Delta t})}{j \Omega b}$ $-\sum_p \frac{\Lambda \epsilon_0 \alpha_p \gamma_p \Delta t e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t)}{j \Omega b} + \frac{\sigma \Lambda}{j \Omega}$	$\Delta t^2 \left(-\sum_p \frac{j \epsilon_0 \beta_p \gamma_p (\alpha_p (2 \alpha_p^2 + 5 j \omega \alpha_p - 4 \omega^2))}{12 d} \right.$ $\left. - \sum_p \frac{j \epsilon_0 \beta_p \gamma_p (\beta_p^2 (2 \alpha_p + j \omega) - 2 j \omega^3)}{12 d} + \frac{j \omega \sigma}{12} \right)$
DE	$\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \gamma \Delta t e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t)}{b} + \frac{\sigma e^{j \omega \Delta t / 2}}{j \Omega}$	$\Delta t \sigma / 2$
PE	$\epsilon_0 \epsilon_\infty + \sum_p \frac{\epsilon_0 \gamma \Delta t e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t)}{b} + \frac{\sigma \Lambda}{j \Omega}$	$\Delta t^2 \left(\sum_p \frac{-\epsilon_0 \beta_p \gamma_p}{12} + \frac{j \omega \sigma}{12} \right)$
JE	$\epsilon_0 \epsilon_\infty + \sum_p \frac{\Lambda \epsilon_0 \beta_p \gamma_p \Delta t (e^{j \omega \Delta t} - e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t))}{j \Omega b}$ $-\sum_p \frac{\Lambda \epsilon_0 \alpha_p \gamma_p \Delta t e^{-\alpha_p \Delta t} \sin(\beta_p \Delta t)}{j \Omega b} + \frac{\sigma \Lambda}{j \Omega}$	$\Delta t \frac{-j \epsilon_0 \beta_p \gamma_p}{2 \omega}$
ADE	$\epsilon_0 \epsilon_\infty + \sum_p \frac{\Lambda^2 \epsilon_0 \beta_p \gamma_p}{\alpha_p^2 + \beta_p^2 + 2 \alpha_p j \Omega \Lambda - \Omega^2} + \frac{\sigma \Lambda}{j \Omega}$	$\Delta t^2 \left(\sum_p \frac{-\omega^2 \epsilon_0 \beta_p \gamma_p (3 \alpha_p^2 + 3 \beta_p^2 + j 2 \alpha_p - 2 \omega^2)}{12 d^2} + \frac{j \omega \sigma}{12} \right)$
$PLRC$ (notations can be found in [27, 91])	$\epsilon_0 \epsilon_\infty - \sum_p \frac{\text{Re}(\hat{\chi}_p^0) \epsilon_0 e^{j \omega \Delta t / 2}}{j \Omega \Delta t} - \sum_p \epsilon_0 \text{Re}(\hat{\epsilon}_p \hat{\chi}_p^0)$ $-\sum_p \frac{(S_1 + S_2) e^{j \omega \Delta t / 2}}{j \Omega \Delta t} + \frac{\sigma \Lambda}{j \Omega}$	$\Delta t^2 \sum_p \frac{-\omega^2 \epsilon_0 \beta_p \gamma_p}{12 d^2}$

$$b = e^{j \omega \Delta t} - 2 e^{-\alpha_p \Delta t} \cos(\beta_p \Delta t) + e^{-2 \alpha_p \Delta t - j \omega \Delta t}, \quad d = \alpha_p^2 + \beta_p^2 + j \omega 2 \alpha_p, \quad \Lambda = \cos(\omega \Delta t / 2)$$

Having tabulated all the relevant complex numerical permittivities, the dispersion relation of (3.9.2) is complete and it can be shown that (3.9.2) converges to the analytical dispersion relation when all the discretizations in time and space are

Figure 3.15: Normalized (a) phase and (b) attenuation errors versus frequency using various formulations for Debye media. ©2009 IEEE.

infinitesimally small. As $\Delta t, \Delta x, \Delta y, \Delta z \rightarrow 0$, $\mathbf{K} \rightarrow \mathbf{k}$, $\Omega \rightarrow \omega$, $\epsilon_{nc} \rightarrow \epsilon(\omega)$ and (3.9.2) reduces to the familiar analytical dispersion relation $\mathbf{k} \cdot \mathbf{k} = \omega^2 \mu_0 \epsilon(\omega)$. It can also be seen that for different methods, ϵ_{nc} converges to analytical $\epsilon(\omega)$ at a different rate due to different order of the leading error term. Obviously, corrected impulse invariance method has the convergence rate twice that of classical impulse invariance method.

3.10 Numerical Results for Corrected Impulse Invariance

The scalar wave numbers k_x , k_y , and k_z of (3.9.2) at each direction can be solved to obtain the dispersion characteristics of a particular method. If only 1D propagation in z -direction is considered, k_z can be expressed explicitly as

$$k_z = \frac{2}{\Delta z} \sin^{-1} \left(\frac{\Delta z \sqrt{\mu_0 \epsilon_{nc}}}{\Delta t} \sin \left(\frac{\omega \Delta t}{2} \right) \right) \quad (3.10.1)$$

Figure 3.16: Normalized (a) phase and (b) attenuation errors versus frequency using various formulations for Lorentz media.

Note that k_z is complex in nature and can be compared to the analytical wave number $k(\omega) = \omega \sqrt{\mu_0 \epsilon(\omega)}$. The real and (negative) imaginary parts of k are associated with the phase and attenuation constants respectively. We further define the normalized phase error as $\left| \frac{\text{Re}(k_{\text{solved}}) - \text{Re}(k_{\text{analytical}})}{\text{Re}(k_{\text{analytical}})} \right|$ and normalized attenuation error as $\left| \frac{\text{Im}(k_{\text{solved}}) - \text{Im}(k_{\text{analytical}})}{\text{Im}(k_{\text{analytical}})} \right|$ to facilitate the analysis.

Fig. 3.15a plots the normalized phase error and Fig. 3.15b the corresponding normalized attenuation error using various formulations for Debye media. The Debye medium considered has three first order poles characterized by $\epsilon_\infty = 4.3$, $\Delta\epsilon_1 = 1970$, $\Delta\epsilon_2 = 30.8$, $\Delta\epsilon_3 = 41.3$, $\tau_1 = 1/(5.2\pi)\mu\text{s}$, $\tau_2 = 1/(680\pi)\mu\text{s}$, $\tau_3 = 1/(46\pi)\text{ns}$ and $\sigma = 5\text{S/m}$ [35]. The conductivity used here has a larger value compared to [35] so that its effect can be demonstrated clearly. The cell size Δz and time step Δt are set at $37.5\mu\text{m}$ and 0.125ps respectively. It can be seen from Fig. 3.15a and Fig. 3.15b that all corrected impulse invariance methods generally yield much lower normalized phase and attenuation errors than all classical impulse invariance methods, and they have approximately the same level of errors exhibited

by ADE and PLRC methods. These again reaffirm the fact that corrected impulse invariance method has higher order of temporal accuracy than classical impulse invariance method. For JE , both normalized phase and attenuation errors increase dramatically as the frequency decreases. This can be understood from its leading error term where it is inversely proportionate to ω as seen from Table 3.8.

Furthermore, we can see that DE has both higher normalized phase and attenuation errors compared to PE . By referring to Table 3.8, it can be seen that the first order leading error term of DE involves additional conductivity term compared to PE , which further degrades the performance. As a matter of fact, although PE has first order leading error term, the error term associated to conductivity is of second order. To explain this, we can see from (3.7.7) that the conversion from frequency to Z domain of PE does not involve conductivity term. Instead, the conductivity term appears in Ampere's law (3.7.8) where central approximation and time averaging are used. On the other hand, the conversion made by DE involves the conductivity term directly as seen from (3.7.2). Therefore, invoking classical impulse invariance method will cause only the DE to have lower order of temporal accuracy for the conductivity term. For clearer illustration, let us refer to the second entry of Table 3.5 which has similar form of frequency domain transfer function as the conductivity term in (3.7.2). The transformation into Z domain using the corrected impulse invariance method is equivalent to taking the central difference approximation with time averaging at time index $n + \frac{1}{2}$. Invoking classical impulse invariance method is seen only as taking the backward difference approximation at time index $n + 1$, which is of one order lower in temporal accuracy. From this, the higher order temporal accuracy of corrected impulse invariance method compared to classical impulse invariance method becomes even more intuitive and apparent.

On the other hand, Fig. 3.16a plots the normalized phase error and Fig. 3.16b the

Figure 3.17: Absolute electric field error versus cell position computed using various formulations of (a) classical and (b) corrected impulse invariance methods for Debye media. ©2009 IEEE.

corresponding normalized attenuation error using various formulations for Lorentz media. The Lorentz medium considered has two second-order poles characterized by $\epsilon_\infty = 1.5$, $\Delta\epsilon_1 = 0.6$, $\Delta\epsilon_2 = 0.9$, $\omega_1 = 40\pi \times 10^9 \text{ rad/s}$, $\omega_2 = 100\pi \times 10^9 \text{ rad/s}$, $\delta_1 = 0.1\omega_1$, $\delta_2 = 0.1\omega_2$ and $\sigma = 5 \text{ S/m}$ [35]. Same as previous Debye media case, the conductivity used here has a larger value compared to [35] so that its effect can be demonstrated clearly. The cell size Δz and time step Δt are set at $37.5 \mu\text{m}$ and 0.125 ps respectively. Again, it can be seen from Fig. 3.16a and Fig. 3.16b that all corrected impulse invariance methods generally yield much lower normalized phase and attenuation errors than all classical impulse invariance methods (except PE), and they have approximately the same level of errors exhibited by ADE and PLRC methods. PE has the same error level as PE_{cor} because no correction is needed in its formulation for Lorentz media discussed earlier.

Next, we consider 1D wave propagation in a homogeneous Debye medium of 1000 cells. The cell size Δz and time step Δt are again set at $37.5 \mu\text{m}$ and 0.125 ps respectively. We consider the characterization of a lossy Debye medium with one

Figure 3.18: Absolute electric field error versus cell position computed using various formulations of (a) JE and (b) DE_{cor} , DE , PE_{cor} , PE , ADE and $PLRC$ methods for Lorentz media.

first order pole, where $\epsilon_{\infty} = 1.8$, $\Delta\epsilon = 79.2$, $\tau = 47\text{ps}$ and $\sigma = 0.1\text{S/m}$. Plane wave propagation is initiated by a hard source Gaussian pulse excitation at initial point. The E field in space is traced after certain time steps and the result can be compared to the analytical solution obtained by numerically integrating the exact frequency domain solution. Fig. 3.17a shows the absolute electric field error versus cell position in the Debye medium, computed using various classical impulse invariance methods after 3000 time steps. Fig. 3.17b on the other hand shows the numerical results obtained by using various corrected impulse invariance methods, as well as ADE and $PLRC$ methods. Note the different scales used in both Y axes, which clearly indicate that all corrected impulse invariance methods achieve lower error than classical impulse invariance methods. From Fig. 3.17b, it is also interesting to observe that in this case, the numerical error of JE_{cor} is the lowest among all, even lower than that of existing ADE and $PLRC$ methods.

We repeat the procedures for 1D wave propagation in a homogeneous Lorentz medium of 5000 cells. The Lorentz media is characterized by $\epsilon_{\infty} = 1.5$, $\Delta\epsilon = 1.5$,

$\omega = 40\pi \times 10^9$ rad/s, $\delta = 0.1\omega$ and $\sigma = 0$. Fig. 3.18a shows the absolute electric field error versus cell position in the Lorentz medium, computed using JE after 6000 time steps and Fig. 3.18b shows the numerical results obtained using DE_{cor} , DE , PE_{cor} , PE , JE_{cor} , ADE and PLRC methods. Under the absence of conductivity ($\sigma = 0$), DE now has the same error as DE_{cor} as evident from Table 3.9. In this case, the only remaining classical impulse invariance method which suffers high inaccuracy is JE .

3.11 Conclusions

This chapter has presented the generalized stability criterion for 3-D FDTD schemes for doubly lossy media, where both electric and magnetic conductivities coexist. The generalized stability criterion is applicable for all FDTD schemes, such as TA, TF, TB and ETD. It is reducible to either electrically lossy, magnetically lossy or lossless media. The stability criterion for PML matching condition can also be obtained as a special case to the doubly lossy media. It has been shown that, for doubly lossy media, the stability criterion for ETD and TF becomes even more relaxed, and for TB, even more stringent compared to either electrically lossy, magnetically lossy or lossless media. On the other hand, the stability criterion for TA remains unchanged even in doubly lossy media. The tunneling of electromagnetic wave through a very thin doubly lossy conductor has been numerically demonstrated. Numerical experiments further show the maximum allowed time step as dictated by the derived stability criterion for different schemes.

Furthermore, this chapter has presented the 3-D dispersion analysis of FDTD schemes for doubly lossy media, where both electric and magnetic conductivities are nonzero. It has been shown that, unlike in electrically lossy media, the attenuation constant in doubly lossy media can be larger than its phase constant. This further calls for care-

ful choice of cell size such that both wavelength and skin depth of the doubly lossy media are properly resolved. From the dispersion analysis, TF generally displays higher phase velocity and attenuation errors due to its first-order temporal accuracy nature compared to second-order ETD and TA. Although both have second-order temporal accuracy, ETD has generally lower phase velocity and attenuation errors than TA. This may be attributed to its closer resemblance to the solution of first-order differential equation. Numerical FDTD simulations in 1-D and 3-D further confirm these findings. Owing to its higher accuracy, ETD should be better than TA for FDTD simulation of doubly lossy or electrically lossy media.

We have also presented the thorough discussions of corrected impulse invariance method in the realm of Z-transform theory for dispersive media. The correction has been shown to be necessary for dispersive media which exhibit discontinuity at $t = 0$ in the time domain susceptibility function. A corrected Z-transform table has been provided to facilitate the conversion from frequency to Z domain. With the aid of the table, various formulations using both corrected and classical impulse invariance methods have been carried out conveniently. Detailed performance measures such as numerical permittivity, leading error term, dispersion relation, normalized phase and attenuation errors as well as memory storage requirements have been included along with some extensive numerical comparisons.

It has been demonstrated that using certain formulation, the corrected impulse invariance method can be potentially more superior compared to existing schemes such as ADE and PLRC methods. It is hoped that this chapter has clearly pointed out the shortcomings that may be encountered by the classical impulse invariance method, and all the corrections necessary for improving the method.

Chapter 4

Unconditionally Stable FADI-FDTD Method for Lossy and Dispersive Media

4.1 Introduction

The ADI-FDTD method [3, 4] has been developed to remove the CFL constraint on the chosen time step, hence the unconditional stability feature. Such feature makes the ADI-FDTD method attractive for further extension into lossy media using different schemes [47–53]. Some stability analysis using the Von Neumann eigenvalue approach has been provided in [51] and [52] for several ADI-FDTD schemes for 1-D and 2-D electrically lossy media. The Von Neumann eigenvalue method, which converts the difference equation into Fourier domain for determining the magnitude of the eigenvalues is straightforward and popular for stability analysis. While this approach is still applicable for lossless ADI-FDTD method, or perhaps simpler specific case of electrically lossy in 1-D or 2-D, it is often tedious in 3-D doubly lossy media (both electric and magnetic conductivities are nonzero) due to the complexity of the updating matrix of the ADI-FDTD schemes.

Of late, the energy-based method has been widely used as an alternative method

to the Von Neumann eigenvalue approach. The unconditionally stable feature of the ADI-FDTD in lossless media has been shown in [86], while the most commonly used averaging scheme of ADI-FDTD method for lossy media is presented in [49]. The matrix norm approach for stability analysis is another viable option which has been applied in lossless Crank-Nicolson, split-step and ADI-FDTD method [87, 88]. Nevertheless, it appears that the full 3-D stability analysis of various possible ADI-FDTD schemes for the most general case of doubly lossy media are still lacking.

In this chapter, we shall present the Lyapunov and matrix norm stability analysis applied to various ADI-FDTD schemes for doubly lossy media. The stability analysis is performed rigorously in both time and Fourier domains. Among the schemes considered are averaging, forward-backward, backward-forward, forward-forward, exponential time differencing and backward-backward (These schemes will be further elaborated in Section 4.4). Averaging, exponential time differencing, forward-backward and backward-forward schemes have second order temporal accuracy. For forward-forward and backward-backward schemes, the temporal accuracy is only of first order. Generally, exponential time differencing has the highest accuracy for its closest resemblance to the solution of first-order differential equation, while averaging scheme is easier to formulate and is most commonly used. Forward-backward and backward-forward schemes, on the other hand, can be used for higher efficiency implementation due to involvement of fewer conductivity terms.

The Lyapunov method, somewhat related to energy-based method, and matrix norm method are ideal stability analysis approaches for various ADI-FDTD schemes due to some unique features in its updating matrices, which will be shown later. For Lyapunov stability analysis, it will be shown that one does not need to solve the discrete Lyapunov equation to deduce the stability of the particular scheme. Instead, one would only require to determine the positive definiteness of a certain matrix. From

there, the subtle relationship between the Lyapunov and energy-based methods can also be seen. On the other hand, the matrix norm stability analysis yields the same condition to ensure stability as the Lyapunov method. Hence, the unconditionally stable feature of various ADI-FDTD schemes is proven. For scheme which is found to be not unconditionally stable, the condition for stability is determined.

Further, we note that the implementation of conventional form of ADI-FDTD method is rather complicated. Apart from solving tridiagonal systems, the RHS of the update equations involve many update coefficients and field variables (resultant from RHS matrix-operators) that require considerable arithmetic operations. Furthermore, one should not overlook the huge amount of memory indexing operations incurred throughout the whole procedures. The introduction of conductivity terms for lossy media into ADI-FDTD algorithm has made such overhead worse from the efficiency point of view where the arithmetic operations and memory indexing increase considerably. Furthermore, it is often desirable to formulate various schemes of ADI-FDTD method under unified schemes which feature higher efficiency and simplicity.

Recently, a new algorithm of efficient ADI-FDTD method [120] which features higher efficiency has been proposed. Such efficient ADI algorithm is included within a family of fundamental implicit schemes, which feature similar fundamental updating structures that are in simplest forms with most efficient matrix-operator-free RHS [121]. Extension of such efficient fundamental form of ADI-FDTD method for lossy media with forward-backward scheme has been discussed in [53], where the conductivity terms are applied at the forward time $(n + \frac{1}{2})$ in the first sub-step and backward time $(n + \frac{1}{2})$ in the second. In this chapter, we consider many more schemes and further unify these schemes based on both conventional form (with RHS matrix-operators) and efficient fundamental form (with RHS matrix-

operator-free) of ADI-FDTD for lossy media. Among the schemes considered are averaging, forward-forward, forward-backward and novel ETD schemes. The novel scheme based on the ETD [7,8] is introduced for the first time (in the main grid) in efficient fundamental form of ADI-FDTD method, which also achieves higher accuracy compared to other schemes. In addition, the implementation of conventional ADI-FDTD method for dispersive media is made complicated by the introduction of additional auxiliary variables. In this chapter, we shall also present the formulation of FADI-FDTD method for various dispersive media. Apart from Debye, Lorentz and Drude models, we also consider the complex conjugate pole-residue pair model. The generalized formulation is shown. Such generalized formulation is applicable to all aforementioned dispersive models.

4.2 Generalized Lyapunov Stability Analysis

Consider a discrete system

$$\mathbf{u}^{n+1} = \mathbf{M}\mathbf{u}^n \quad (4.2.1)$$

where $\mathbf{u}$ is the state vector with time indices n and $n+1$, and $\mathbf{M}$ is the amplification matrix. The system is said to be stable in the sense of Lyapunov if the state vector remains bounded near the origin for all $n \geq 0$. Furthermore, if the state vector converges to the origin as $n \rightarrow \infty$, the system is asymptotically stable. The Lyapunov theorem states that the above discrete system is stable in the sense of Lyapunov if there exists a positive definite $\mathbf{Q}$ to the discrete Lyapunov equation

$$\mathbf{M}^T \mathbf{Q} \mathbf{M} - \mathbf{Q} = -\mathbf{P} \quad (4.2.2)$$

such that $\mathbf{P}$ is positive semidefinite. If there exists a positive definite $\mathbf{Q}$ to (4.2.2) such that $\mathbf{P}$ is positive definite, the system is asymptotically stable [115–117]. In

FDTD stability analysis, researchers are often interested in whether the solution will always remain bounded (nonincreasing) as the time marches. Therefore, it should be mentioned that throughout the chapter, if the system is found to be either stable in the sense of Lyapunov, or asymptotically stable, we shall simply refer them as “stable”.

In the following, the above Lyapunov theorem will be applied in the stability analysis of ADI-FDTD schemes for doubly lossy media. The discretized Maxwell equations in space describing an electromagnetics problem within a computational domain terminated by PEC walls can be expressed in compact matrix form as

$$\frac{\partial}{\partial t} \begin{bmatrix} \mathbf{D}_\epsilon & \mathbf{O} \\ \mathbf{O} & \mathbf{D}_\mu \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix} = \begin{bmatrix} \mathbf{D}_\sigma & -\mathbf{C}^T \\ \mathbf{C} & \mathbf{D}_{\sigma^*} \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix} \quad (4.2.3)$$

where

$$\mathbf{e} = \begin{bmatrix} E_{x(i+\frac{1}{2},j,k)} & E_{y(i,j+\frac{1}{2},k)} & E_{z(i,j,k+\frac{1}{2})} \end{bmatrix}^T \quad (4.2.4)$$

$$\mathbf{h} = \begin{bmatrix} H_{x(i,j+\frac{1}{2},k+\frac{1}{2})} & H_{y(i+\frac{1}{2},j,k+\frac{1}{2})} & H_{z(i+\frac{1}{2},j+\frac{1}{2},k)} \end{bmatrix}^T \quad (4.2.5)$$

$$\mathbf{D}_\epsilon = \text{diag} \left(\epsilon_{x(i+\frac{1}{2},j,k)}, \epsilon_{y(i,j+\frac{1}{2},k)}, \epsilon_{z(i,j,k+\frac{1}{2})} \right) \quad (4.2.6)$$

$$\mathbf{D}_\mu = \text{diag} \left(\mu_{x(i,j+\frac{1}{2},k+\frac{1}{2})}, \mu_{y(i+\frac{1}{2},j,k+\frac{1}{2})}, \mu_{z(i+\frac{1}{2},j+\frac{1}{2},k)} \right) \quad (4.2.7)$$

$$\mathbf{D}_\sigma = \text{diag} \left(\sigma_{x(i+\frac{1}{2},j,k)}, \sigma_{y(i,j+\frac{1}{2},k)}, \sigma_{z(i,j,k+\frac{1}{2})} \right) \quad (4.2.8)$$

$$\mathbf{D}_{\sigma^*} = \text{diag} \left(\sigma_{x(i,j+\frac{1}{2},k+\frac{1}{2})}^*, \sigma_{y(i+\frac{1}{2},j,k+\frac{1}{2})}^*, \sigma_{z(i+\frac{1}{2},j+\frac{1}{2},k)}^* \right). \quad (4.2.9)$$

Note that i , j and k are grid position indices within the whole computation domain along x , y and z directions, respectively. $\mathbf{C}$ is the curl matrix comprising spatial step Δx , Δy and Δz resulting from the discretization of the curl operator through central differencing approximation. $\mathbf{O}$ is the null matrix. The dimensions of all matrices and vectors are dependent on the size of the computational domain. Henceforth, the indices i , j , k of material parameters ϵ , μ , σ and σ^* shall be dropped for convenience.

Upon discretizing in time, the ADI-FDTD update equations for doubly lossy media generally read:

$$(\mathbf{I} + \mathbf{D}_A - \mathbf{D}_C \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I} - \mathbf{D}_B + \mathbf{D}_C \mathbf{B}) \mathbf{u}^n \quad (4.2.10a)$$

$$(\mathbf{I} + \mathbf{D}_B - \mathbf{D}_C \mathbf{B}) \mathbf{u}^{n+1} = (\mathbf{I} - \mathbf{D}_A + \mathbf{D}_C \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} \quad (4.2.10b)$$

where

$$\mathbf{u} = \begin{bmatrix} \mathbf{e} & \mathbf{h} \end{bmatrix}^T \quad (4.2.11)$$

$$\mathbf{A} = \begin{bmatrix} \mathbf{O} & -\mathbf{C}_1^T \\ \mathbf{C}_1 & \mathbf{O} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} \mathbf{O} & -\mathbf{C}_2^T \\ \mathbf{C}_2 & \mathbf{O} \end{bmatrix}. \quad (4.2.12)$$

$\mathbf{I}$ is identity matrix with dimension dependent on the size of computational domain.

$\mathbf{C}_1$ and $\mathbf{C}_2$ are composed of discretization coefficients of spatial derivatives matrices

$\begin{bmatrix} 0 & 0 & \partial/\partial y \\ \partial/\partial z & 0 & 0 \\ 0 & \partial/\partial x & 0 \end{bmatrix}$ and $\begin{bmatrix} 0 & -\partial/\partial z & 0 \\ 0 & 0 & -\partial/\partial x \\ -\partial/\partial y & 0 & 0 \end{bmatrix}$, respectively. Their dimensions are also dependent on the size of computational domain. Note that $\mathbf{C}_1$ and $\mathbf{C}_2$

are split from $\mathbf{C} = \mathbf{C}_1 + \mathbf{C}_2$ such that they yield computationally efficient tridiagonal matrices in both substeps of (4.2.10). $\mathbf{D}_A$, $\mathbf{D}_B$ and $\mathbf{D}_C$ are all diagonal matrices which comprise Δt , and material parameters matrices $\mathbf{D}_\epsilon$, $\mathbf{D}_\mu$, $\mathbf{D}_\sigma$ and $\mathbf{D}_{\sigma^*}$. For the moment, we shall let matrices $\mathbf{D}_A$, $\mathbf{D}_B$ and $\mathbf{D}_C$ be general but they will be further defined accordingly for different schemes in the subsequent sections.

Before the discrete Lyapunov equation is applied, the following transformation of vector

$$\mathbf{v} = \mathbf{D}_C^{-\frac{1}{2}} \mathbf{u} \quad (4.2.13)$$

is used to yield the overall ADI-FDTD update equations of

$$\begin{aligned}\mathbf{v}^{n+1} &= (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)^{-1} (\mathbf{I} - \mathbf{D}_A + \mathbf{A}_C) (\mathbf{I} + \mathbf{D}_A - \mathbf{A}_C)^{-1} (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C) \mathbf{v}^n \\ &= \mathbf{M} \mathbf{v}^n\end{aligned}\quad (4.2.14)$$

where

$$\mathbf{A}_C = \mathbf{D}_C^{\frac{1}{2}} \mathbf{A} \mathbf{D}_C^{\frac{1}{2}} \quad (4.2.15)$$

$$\mathbf{B}_C = \mathbf{D}_C^{\frac{1}{2}} \mathbf{B} \mathbf{D}_C^{\frac{1}{2}}. \quad (4.2.16)$$

Note that as long as we can find a pair of positive definite (or positive semidefinite) $\mathbf{P}$ and positive definite $\mathbf{Q}$ satisfying (4.2.2), the sufficiency for stability is guaranteed.

To that end, we choose $\mathbf{Q}$ as

$$\mathbf{Q} = (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)^T (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C). \quad (4.2.17)$$

An arbitrary vector $\mathbf{v}$ and its transpose $\mathbf{v}^T$ are multiplied from the left and right at both sides of (4.2.2) to yield an energy-like equation

$$(\mathbf{v}^n)^T \mathbf{M}^T \mathbf{Q} \mathbf{M} \mathbf{v}^n - (\mathbf{v}^n)^T \mathbf{Q} \mathbf{v}^n = -(\mathbf{v}^n)^T \mathbf{P} \mathbf{v}^n. \quad (4.2.18)$$

Noting that $\mathbf{v}^{n+1} = \mathbf{M} \mathbf{v}^n$, (4.2.18) is rewritten as

$$(\mathbf{v}^{n+1})^T \mathbf{Q} \mathbf{v}^{n+1} - (\mathbf{v}^n)^T \mathbf{Q} \mathbf{v}^n = -(\mathbf{v}^n)^T \mathbf{P} \mathbf{v}^n. \quad (4.2.19)$$

Substituting $\mathbf{Q}$ in (4.2.17) into (4.2.19) and upon some manipulation, one obtains

$$\begin{aligned}& (\mathbf{v}^{n+1})^T (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)^T (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C) \mathbf{v}^{n+1} \\ & - (\mathbf{v}^n)^T (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C)^T (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C) \mathbf{v}^n \\ & - [(\mathbf{v}^n)^T (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)^T (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C) \mathbf{v}^n \\ & - (\mathbf{v}^n)^T (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C)^T (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C) \mathbf{v}^n]\end{aligned}$$

$$= -(\mathbf{v}^n)^T \mathbf{P} \mathbf{v}^n. \quad (4.2.20)$$

From ADI-FDTD update procedures, we know that

$$(\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C) \mathbf{v}^{n+1} = (\mathbf{I} - \mathbf{D}_A + \mathbf{A}_C) \mathbf{v}^{n+\frac{1}{2}} \quad (4.2.21)$$

$$(\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C) \mathbf{v}^n = (\mathbf{I} + \mathbf{D}_A - \mathbf{A}_C) \mathbf{v}^{n+\frac{1}{2}}. \quad (4.2.22)$$

Substituting these into the first two terms of above equation, one gets

$$\begin{aligned} & (\mathbf{v}^{n+\frac{1}{2}})^T (\mathbf{I} - \mathbf{D}_A + \mathbf{A}_C)^T (\mathbf{I} - \mathbf{D}_A + \mathbf{A}_C) \mathbf{v}^{n+\frac{1}{2}} \\ & - (\mathbf{v}^{n+\frac{1}{2}})^T (\mathbf{I} + \mathbf{D}_A - \mathbf{A}_C)^T (\mathbf{I} + \mathbf{D}_A - \mathbf{A}_C) \mathbf{v}^{n+\frac{1}{2}} \\ & - [(\mathbf{v}^n)^T (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)^T (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C) \mathbf{v}^n \\ & - (\mathbf{v}^n)^T (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C)^T (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C) \mathbf{v}^n] \\ & = -(\mathbf{v}^n)^T \mathbf{P} \mathbf{v}^n. \end{aligned} \quad (4.2.23)$$

Noting that $\mathbf{A}_C$ and $\mathbf{B}_C$ are skew-symmetric ($\mathbf{A}_C = -\mathbf{A}_C^T$ and $\mathbf{B}_C = -\mathbf{B}_C^T$), (4.2.23) is reduced into

$$(\mathbf{v}^{n+\frac{1}{2}})^T 4(-\mathbf{D}_A) \mathbf{v}^{n+\frac{1}{2}} - (\mathbf{v}^n)^T 4\mathbf{D}_B \mathbf{v}^n = -(\mathbf{v}^n)^T \mathbf{P} \mathbf{v}^n. \quad (4.2.24)$$

Taking into consideration the relationship between $\mathbf{v}^{n+\frac{1}{2}}$ and $\mathbf{v}^n$ in (4.2.22), one finally arrives at

$$(\mathbf{v}^n)^T \mathbf{Y}^T 4(-\mathbf{D}_A) \mathbf{Y} \mathbf{v}^n - (\mathbf{v}^n)^T 4\mathbf{D}_B \mathbf{v}^n = -(\mathbf{v}^n)^T \mathbf{P} \mathbf{v}^n \quad (4.2.25)$$

where $\mathbf{Y} = (\mathbf{I} + \mathbf{D}_A - \mathbf{A}_C)^{-1} (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C)$.

Thus, $\mathbf{P}$ is finally derived as

$$\mathbf{P} = 4 \left(\mathbf{Y}^T \mathbf{D}_A \mathbf{Y} + \mathbf{D}_B \right). \quad (4.2.26)$$

The first term inside the bracket in (4.2.26) preserves the definiteness of $\mathbf{D}_A$. Hence, if $\mathbf{D}_A$ and $\mathbf{D}_B$ are positive definite (positive semidefinite), $\mathbf{P}$ is positive definite (positive semidefinite). A positive definite or semidefinite $\mathbf{P}$ implies that the energy of the system is always bounded and stability is ensured. Furthermore, the specified $\mathbf{Q}$ in (4.2.17) is always positive definite for nonsingular $(\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)$ (otherwise the whole amplification matrix $\mathbf{M}$ in (4.2.14) is undefined) [118]. Therefore, the sufficient condition for stability of ADI-FDTD schemes for doubly lossy media is such that $\mathbf{D}_A$ and $\mathbf{D}_B$ are positive definite or positive semidefinite. Note that $\mathbf{D}_C$ has no bearing over the stability of the ADI-FDTD schemes.

4.3 Generalized Matrix Norm Stability Analysis

For the same discrete system in (4.2.1), $\mathbf{u}$ will always be bounded (stable) as the time marches if we can find any induced matrix norm (e.g. 1-norm, 2-norm, ∞ -norm) to the amplification matrix, $\mathbf{M}$ such that $\|\mathbf{M}\| \leq 1$ [119].

For matrix norm analysis, we proceed from (4.2.14) and apply transformation vector of

$$\mathbf{w} = (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C) \mathbf{v} \quad (4.3.1)$$

to yield

$$\begin{aligned} \mathbf{w}^{n+1} &= (\mathbf{I} - \mathbf{D}_A + \mathbf{A}_C) (\mathbf{I} + \mathbf{D}_A - \mathbf{A}_C)^{-1} (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C) (\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)^{-1} \mathbf{w}^n \\ &= \mathbf{M}' \mathbf{w}^n \\ &= \mathbf{M}_A \mathbf{M}_B \mathbf{w}^n \end{aligned} \quad (4.3.2)$$

where

$$\mathbf{M}_A = (\mathbf{I} - \mathbf{D}_A + \mathbf{A}_C) (\mathbf{I} + \mathbf{D}_A - \mathbf{A}_C)^{-1} \quad (4.3.3)$$

$$\mathbf{M}_B = (\mathbf{I} - \mathbf{D}_B + \mathbf{B}_C)(\mathbf{I} + \mathbf{D}_B - \mathbf{B}_C)^{-1}. \quad (4.3.4)$$

It should be noted that evaluating the matrix norm directly from $\mathbf{M}$ in (4.2.14) is difficult. The rationale behind transforming $\mathbf{v}$ further into $\mathbf{w}$ in (4.3.1) is to transform $\mathbf{M}$ in (4.2.14) into $\mathbf{M}'$ in (4.3.2). $\mathbf{M}_A$ and $\mathbf{M}_B$ can then be extracted and their respective norm can be evaluated separately.

From the definition of induced matrix norm, the 2-norm (euclidean norm) of $\mathbf{M}_A$ can be expressed as

$$\|\mathbf{M}_A\|_2 = \sqrt{\sup_{\forall \mathbf{x}, \mathbf{x} \neq 0} \frac{[(\mathbf{I} - \mathbf{T}_A) \mathbf{x}]^T (\mathbf{I} - \mathbf{T}_A) \mathbf{x}}{[(\mathbf{I} + \mathbf{T}_A) \mathbf{x}]^T (\mathbf{I} + \mathbf{T}_A) \mathbf{x}}} \quad (4.3.5)$$

where $\mathbf{T}_A = \mathbf{D}_A - \mathbf{A}_C$.

Since $\mathbf{A}_C$ is skew-symmetric ($\mathbf{A}_C = -\mathbf{A}_C^T$), (4.3.5) can be reduced into

$$\|\mathbf{M}_A\|_2 = \sqrt{\sup_{\forall \mathbf{x}, \mathbf{x} \neq 0} \frac{\mathbf{x}^T [(\mathbf{I} - \mathbf{D}_A)^T (\mathbf{I} - \mathbf{D}_A) + \mathbf{R}_A] \mathbf{x}}{\mathbf{x}^T [(\mathbf{I} + \mathbf{D}_A)^T (\mathbf{I} + \mathbf{D}_A) + \mathbf{R}_A] \mathbf{x}}} \quad (4.3.6)$$

where $\mathbf{R}_A = \mathbf{A}_C^T \mathbf{A}_C - \mathbf{A}_C^T \mathbf{D}_A - \mathbf{D}_A \mathbf{A}_C$. We can see from (4.3.6) that if $\mathbf{D}_A$ is positive definite or positive semidefinite, $(\mathbf{I} - \mathbf{D}_A)^T (\mathbf{I} - \mathbf{D}_A) \leq (\mathbf{I} + \mathbf{D}_A)^T (\mathbf{I} + \mathbf{D}_A)$, and thus, $\|\mathbf{M}_A\|_2 \leq 1$.

Similarly, by replacing $\mathbf{A}_C$ with $\mathbf{B}_C$ and taking the skew-symmetric nature of $\mathbf{B}_C$ ($\mathbf{B}_C = -\mathbf{B}_C^T$) into consideration, we obtain

$$\|\mathbf{M}_B\|_2 = \sqrt{\sup_{\forall \mathbf{x}, \mathbf{x} \neq 0} \frac{\mathbf{x}^T [(\mathbf{I} - \mathbf{D}_B)^T (\mathbf{I} - \mathbf{D}_B) + \mathbf{R}_B] \mathbf{x}}{\mathbf{x}^T [(\mathbf{I} + \mathbf{D}_B)^T (\mathbf{I} + \mathbf{D}_B) + \mathbf{R}_B] \mathbf{x}}} \quad (4.3.7)$$

where $\mathbf{R}_B = \mathbf{B}_C^T \mathbf{B}_C - \mathbf{B}_C^T \mathbf{D}_B - \mathbf{D}_B \mathbf{B}_C$. Here, $\|\mathbf{M}_B\|_2 \leq 1$ if $\mathbf{D}_B$ is positive definite or positive semidefinite.

Using norm inequality of

$$\|\mathbf{M}'\|_2 \leq \|\mathbf{M}_A\|_2 \cdot \|\mathbf{M}_B\|_2, \quad (4.3.8)$$

we note that both $\|\mathbf{M}_A\|_2 \leq 1$ and $\|\mathbf{M}_B\|_2 \leq 1$ imply that $\|\mathbf{M}'\|_2 \leq 1$, which guarantees stability. It can be seen that the condition to guarantee algorithm stability formulated from matrix norm stability analysis is exactly the same as those formulated from Lyapunov stability analysis in the previous section. Both analyses show that the positive definiteness (or positive semidefiniteness) of $\mathbf{D}_A$ and $\mathbf{D}_B$ are paramount to ensure stability of ADI-FDTD schemes for doubly lossy media.

4.4 Stability Analysis of Various ADI-FDTD Schemes for Doubly Lossy Media

We now proceed to analyze the stability of various ADI-FDTD schemes for doubly lossy media using the above generalized stability analysis. The schemes considered in this section include averaging, forward-backward, backward-forward, exponential time differencing, forward-forward, backward-backward and lossless ADI-FDTD.

4.4.1 Averaging

The averaging scheme [47, 49] of ADI-FDTD method for doubly lossy media is one of the most common schemes used where the conductivity terms are averaged between two time indices in both substeps. The scheme calls for the following update procedures:

$$\left(\mathbf{I} + \frac{\Delta t}{4} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}} = \left(\mathbf{I} - \frac{\Delta t}{4} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^n \quad (4.4.1a)$$

$$\left(\mathbf{I} + \frac{\Delta t}{4} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^{n+1} = \left(\mathbf{I} - \frac{\Delta t}{4} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}} \quad (4.4.1b)$$

where

$$\mathbf{D}_{\epsilon\mu} = \begin{bmatrix} \mathbf{D}_\epsilon & \mathbf{O} \\ \mathbf{O} & \mathbf{D}_\mu \end{bmatrix}, \quad \mathbf{D}_{\sigma\sigma^*} = \begin{bmatrix} \mathbf{D}_\sigma & \mathbf{O} \\ \mathbf{O} & \mathbf{D}_{\sigma^*} \end{bmatrix}. \quad (4.4.2)$$

Note that the averaging scheme is second-order in temporal accuracy.

Comparing (4.4.1) to (4.2.10) in the generalized stability analysis, it is found that

$$\mathbf{D}_A = \mathbf{D}_B = \frac{\Delta t}{4} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \quad (4.4.3)$$

$$\mathbf{D}_C = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1}. \quad (4.4.4)$$

If ϵ_ξ , μ_ξ , σ_ξ , σ_ξ^* ($\xi = x, y, z$) of all grid points (inhomogeneous media) within the computational domain and Δt are positive, $\mathbf{D}_A$ and $\mathbf{D}_B$ are always positive definite. Note that σ_ξ and σ_ξ^* can also be zero at certain grid points to represent combination of lossless and lossy media, or electrically lossy ($\sigma^* = 0$) and magnetically lossy ($\sigma = 0$) media likewise. In this case, $\mathbf{D}_A$ and $\mathbf{D}_B$ are always positive semidefinite. As far as Lyapunov stability analysis is concerned, we can see from (4.2.26) that $\mathbf{P}$ is always positive definite, or positive semidefinite. This implies that the energy of the system is always bounded. On the other hand, from matrix norm stability analysis, it can be found from (4.3.6) and (4.3.7) that

$$\|M_A\|_2 \leq 1, \quad \|M_B\|_2 \leq 1 \quad (4.4.5)$$

always hold as long as $\mathbf{D}_A$ and $\mathbf{D}_B$ are positive definite or positive semidefinite.

Therefore, it can be concluded concurrently from both Lyapunov and matrix norm stability analysis that the averaging scheme is unconditionally stable as there is no restriction imposed on the chosen time step Δt .

4.4.2 Forward-Backward

In forward-backward scheme [53], the conductivity terms are applied at the forward time $(n + \frac{1}{2})$ in the first substep and backward time $(n + \frac{1}{2})$ in the second. The

scheme calls for the following update procedures:

$$\left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^n \quad (4.4.6a)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^{n+1} = \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}}. \quad (4.4.6b)$$

The forward-backward scheme is second-order in temporal accuracy.

Comparing (4.4.6) to (4.2.10) in the generalized stability analysis, it is found that

$$\mathbf{D}_A = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \quad (4.4.7)$$

$$\mathbf{D}_B = \mathbf{O} \quad (4.4.8)$$

$$\mathbf{D}_C = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1}. \quad (4.4.9)$$

Here, similar arguments as in the averaging scheme applies. $\mathbf{D}_A$ and $\mathbf{D}_B$ are either always positive definite or positive semidefinite. As a result, from Lyapunov stability analysis, $\mathbf{P}$ is always positive definite or positive semidefinite. This implies that the energy of the system is always bounded. From matrix norm stability analysis, we also find that

$$\|M_A\|_2 \leq 1, \quad \|M_B\|_2 = 1 \quad (4.4.10)$$

always hold as long as $\mathbf{D}_A$ and $\mathbf{D}_B$ are positive definite or positive semidefinite. Therefore, forward-backward scheme is also unconditionally stable.

4.4.3 Backward-Forward

The backward-forward scheme is essentially a dual of the forward-backward scheme. In this scheme, the conductivity terms are applied at the backward time (n) in the first substep and forward time ($n+1$) in the second. The scheme calls for the

following update procedures:

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}} = \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^n \quad (4.4.11a)$$

$$\left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}}. \quad (4.4.11b)$$

The backward-forward scheme is second-order in temporal accuracy.

Comparing (4.4.11) to (4.2.10) in the generalized stability analysis, it is found that

$$\mathbf{D}_A = \mathbf{O} \quad (4.4.12)$$

$$\mathbf{D}_B = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \quad (4.4.13)$$

$$\mathbf{D}_C = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1}. \quad (4.4.14)$$

Again, $\mathbf{D}_A$ and $\mathbf{D}_B$ are either always positive definite or positive semidefinite. As a result, from Lyapunov stability analysis, $\mathbf{P}$ is always positive definite or positive semidefinite. This implies that the energy of the system is always bounded. From matrix norm stability analysis, we also find that

$$\|M_A\|_2 = 1, \quad \|M_B\|_2 \leq 1 \quad (4.4.15)$$

always hold as long as $\mathbf{D}_A$ and $\mathbf{D}_B$ are positive definite or positive semidefinite. Therefore, backward-forward scheme is also unconditionally stable.

4.4.4 Exponential Time Differencing

Apart from being adopted in Yee's explicit FDTD scheme [8], the ETD scheme can also be incorporated into the ADI-FDTD method, which calls for the following update procedures:

$$(\mathbf{I} - \mathbf{D}_e \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} = \left(e^{-\frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*}} + \mathbf{D}_e \mathbf{B}\right) \mathbf{u}^n \quad (4.4.16a)$$

$$(\mathbf{I} - \mathbf{D}_e \mathbf{B}) \mathbf{u}^{n+1} = \left(e^{-\frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*}} + \mathbf{D}_e \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}} \quad (4.4.16b)$$

where $\mathbf{D}_e = \mathbf{D}_{\sigma\sigma^*}^{-1} \left(\mathbf{I} - e^{-\frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*}} \right)$ is diagonal. The ETD scheme is also second-order in temporal accuracy.

Note that the general stability analysis procedure in the previous sections cannot be applied directly to (4.4.16). In order to apply the analysis procedure, we have to first consider the following mapping of matrices:

$$e^{-\frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*}} = (\mathbf{I} + \mathbf{D}_{m1})^{-1} (\mathbf{I} - \mathbf{D}_{m1}). \quad (4.4.17)$$

Using the above mapping along with some manipulation, (4.4.16) can be rewritten as

$$(\mathbf{I} + \mathbf{D}_{m1} - \mathbf{D}_e (\mathbf{I} + \mathbf{D}_{m1}) \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I} - \mathbf{D}_{m1} + \mathbf{D}_e (\mathbf{I} + \mathbf{D}_{m1}) \mathbf{B}) \mathbf{u}^n \quad (4.4.18a)$$

$$(\mathbf{I} + \mathbf{D}_{m1} - \mathbf{D}_e (\mathbf{I} + \mathbf{D}_{m1}) \mathbf{B}) \mathbf{u}^{n+1} = (\mathbf{I} - \mathbf{D}_{m1} + \mathbf{D}_e (\mathbf{I} + \mathbf{D}_{m1}) \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} \quad (4.4.18b)$$

Comparing (4.4.18) to (4.2.10), we obtain

$$\mathbf{D}_A = \mathbf{D}_B = \mathbf{D}_{m1} \quad (4.4.19)$$

$$\mathbf{D}_C = \mathbf{D}_e (\mathbf{I} + \mathbf{D}_{m1}) \quad (4.4.20)$$

where $\mathbf{D}_{m1}$ can be solved from (4.4.17) as

$$\mathbf{D}_{m1} = \left(\mathbf{I} + e^{-\frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*}} \right)^{-1} \left(\mathbf{I} - e^{-\frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*}} \right). \quad (4.4.21)$$

We can see from (4.4.21) that $\mathbf{D}_{m1}$ and hence, $\mathbf{D}_A$ and $\mathbf{D}_B$ are always positive definite or positive semidefinite. As a result, from Lyapunov stability analysis, $\mathbf{P}$ is always positive definite or positive semidefinite. This implies that the energy of the system is always bounded. From matrix norm stability analysis, we also find that

$$\|M_A\|_2 \leq 1, \quad \|M_B\|_2 \leq 1 \quad (4.4.22)$$

always hold as long as $\mathbf{D}_A$ and $\mathbf{D}_B$ are positive definite or positive semidefinite. Therefore, the ETD scheme is unconditionally stable.

4.4.5 Forward-Forward

In forward-forward scheme [50], the conductivity terms are applied at forward time for both substeps ($n + \frac{1}{2}$ for the first and $n + 1$ for second). The scheme calls for the following update procedures:

$$\left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A} \right) \mathbf{u}^{n+\frac{1}{2}} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B} \right) \mathbf{u}^n \quad (4.4.23a)$$

$$\left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B} \right) \mathbf{u}^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A} \right) \mathbf{u}^{n+\frac{1}{2}}. \quad (4.4.23b)$$

Note however that forward-forward scheme is only first-order in temporal accuracy.

In forward-forward scheme, we now consider the mapping of

$$\left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \right)^{-1} = (\mathbf{I} + \mathbf{D}_{m2})^{-1} (\mathbf{I} - \mathbf{D}_{m2}). \quad (4.4.24)$$

Using the above mapping along with some manipulation, (4.4.23) can be rewritten as

$$(\mathbf{I} + \mathbf{D}_{m2} - \mathbf{D}_f (\mathbf{I} + \mathbf{D}_{m2}) \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I} - \mathbf{D}_{m2} + \mathbf{D}_f (\mathbf{I} + \mathbf{D}_{m2}) \mathbf{B}) \mathbf{u}^n \quad (4.4.25a)$$

$$(\mathbf{I} + \mathbf{D}_{m2} - \mathbf{D}_f (\mathbf{I} + \mathbf{D}_{m2}) \mathbf{B}) \mathbf{u}^{n+1} = (\mathbf{I} - \mathbf{D}_{m2} + \mathbf{D}_f (\mathbf{I} + \mathbf{D}_{m2}) \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} \quad (4.4.25b)$$

where $\mathbf{D}_f = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \right)^{-1}$.

Comparing (4.4.25) to (4.2.10), it is observed that

$$\mathbf{D}_A = \mathbf{D}_B = \mathbf{D}_{m2} \quad (4.4.26)$$

$$\mathbf{D}_C = \mathbf{D}_f (\mathbf{I} + \mathbf{D}_{m2}) \quad (4.4.27)$$

where $\mathbf{D}_{m2}$ can be solved from (4.4.24) as

$$\mathbf{D}_{m2} = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \left(2\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \right)^{-1}. \quad (4.4.28)$$

Equation (4.4.28) indicates that $\mathbf{D}_{m2}$ and hence, $\mathbf{D}_A$ and $\mathbf{D}_B$ are always positive definite or positive semidefinite. As a result, from Lyapunov stability analysis, $\mathbf{P}$ is always positive definite or positive semidefinite. This implies that the energy of the system is always bounded. From matrix norm stability analysis, we also find that

$$\|M_A\|_2 \leq 1, \quad \|M_B\|_2 \leq 1 \quad (4.4.29)$$

always hold as long as $\mathbf{D}_A$ and $\mathbf{D}_B$ are positive definite or positive semidefinite. Therefore, the forward-forward scheme is unconditionally stable.

4.4.6 Backward-Backward

In backward-backward scheme, the conductivity terms are applied at backward time for both substeps (n for the first and $n + \frac{1}{2}$ for second). The scheme calls for the following update procedures:

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A} \right) \mathbf{u}^{n+\frac{1}{2}} = \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B} \right) \mathbf{u}^n \quad (4.4.30a)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B} \right) \mathbf{u}^{n+1} = \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A} \right) \mathbf{u}^{n+\frac{1}{2}}. \quad (4.4.30b)$$

In backward-backward scheme, we consider the following mapping of

$$\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu} \mathbf{D}_{\sigma\sigma^*} = (\mathbf{I} + \mathbf{D}_{m3})^{-1} (\mathbf{I} - \mathbf{D}_{m3}). \quad (4.4.31)$$

Note that the mapping applied to backward-backward scheme, c.f. (4.4.31), as well as the mappings applied to ETD and forward-forward schemes in the previous subsections, c.f. (4.4.17) and (4.4.24) are used to transform their update equations into the form of (4.2.10).

Using the above mapping along with some manipulation, (4.4.30) can be written as

$$(\mathbf{I} + \mathbf{D}_{m3} - \mathbf{D}_g (\mathbf{I} + \mathbf{D}_{m3}) \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I} - \mathbf{D}_{m3} + \mathbf{D}_g (\mathbf{I} + \mathbf{D}_{m3}) \mathbf{B}) \mathbf{u}^n \quad (4.4.32a)$$

$$(\mathbf{I} + \mathbf{D}_{m3} - \mathbf{D}_g (\mathbf{I} + \mathbf{D}_{m3}) \mathbf{B}) \mathbf{u}^{n+1} = (\mathbf{I} - \mathbf{D}_{m3} + \mathbf{D}_g (\mathbf{I} + \mathbf{D}_{m3}) \mathbf{A}) \mathbf{u}^{n+\frac{1}{2}} \quad (4.4.32b)$$

where $\mathbf{D}_g = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1}$.

Comparing (4.4.32) to (4.2.10), it is observed that

$$\mathbf{D}_A = \mathbf{D}_B = \mathbf{D}_{m3} \quad (4.4.33)$$

$$\mathbf{D}_C = \mathbf{D}_g (\mathbf{I} + \mathbf{D}_{m3}) \quad (4.4.34)$$

where $\mathbf{D}_{m3}$ can be solved from (4.4.31) as

$$\mathbf{D}_{m3} = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \left(2\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \right)^{-1}. \quad (4.4.35)$$

However, in this case, we can see from (4.4.35) that $\mathbf{D}_{m3}$, and hence $\mathbf{D}_A$ and $\mathbf{D}_B$ are not always positive definite or positive semidefinite even when ϵ_ξ , μ_ξ , σ_ξ , σ_ξ^* of all grid points and Δt are positive. Therefore, backward-backward scheme is not unconditionally stable from Lyapunov stability analysis as $\mathbf{P}$ is not always positive definite or positive semidefinite. In order to ensure positive definiteness or positive semidefiniteness of $\mathbf{D}_{m3}$, the following condition must hold:

$$\left(2\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{D}_{\sigma\sigma^*} \right)^{-1} > 0. \quad (4.4.36)$$

From (4.4.36), we can see that the choice of Δt is somehow bounded by ϵ_ξ , μ_ξ , σ_ξ and σ_ξ^* within the computational domain. Solving (4.4.36) for Δt , the condition to ensure stability for backward-backward scheme is thus given by

$$\Delta t < 4 \left(\min_{\xi=x,y,z,\forall i,\forall j,\forall k} \left\{ \frac{\epsilon_\xi}{\sigma_\xi}, \frac{\mu_\xi}{\sigma_\xi^*} \right\} \right) \quad (4.4.37)$$

where ϵ_ξ , μ_ξ , σ_ξ , σ_ξ^* and Δt are all positive. Equation (4.4.37) implies that the time step should sufficiently resolve the minimum relaxation time of the medium. It should be pointed out that unlike the Yee's explicit FDTD method, the stability criterion of backward-backward scheme of ADI-FDTD is only dependent on the relaxation time of the medium and *independent* of the mesh size.

From matrix norm stability analysis, we now find that

$$\|M_A\|_2 \leq 1, \quad \|M_B\|_2 \leq 1 \quad (4.4.38)$$

only hold if the condition in (4.4.37) is satisfied.

4.4.7 Lossless

For completeness, the stability analysis for the lossless ADI-FDTD method is performed in the realm of Lyapunov and matrix norm stability. The lossless ADI-FDTD method calls for the following update procedures:

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^n \quad (4.4.39a)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{B}\right) \mathbf{u}^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1} \mathbf{A}\right) \mathbf{u}^{n+\frac{1}{2}}. \quad (4.4.39b)$$

It can be seen that

$$\mathbf{D}_A = \mathbf{D}_B = \mathbf{O} \quad (4.4.40)$$

$$\mathbf{D}_C = \frac{\Delta t}{2} \mathbf{D}_{\epsilon\mu}^{-1}. \quad (4.4.41)$$

Due to skew-symmetric nature of $\mathbf{A}_C$, we find that $(\mathbf{I} + \mathbf{A}_C)(\mathbf{I} - \mathbf{A}_C)^{-1}$ is in fact Cayley transform matrix which is orthogonal. Thus, matrix $\mathbf{P}$ can be determined directly from the Lyapunov equation. The Lyapunov equation for lossless ADI-

FDTD read:

$$\begin{aligned}\mathbf{M}^T \mathbf{Q} \mathbf{M} - \mathbf{Q} &= (\mathbf{I} + \mathbf{B}_C)^T (\mathbf{I} + \mathbf{B}_C) - (\mathbf{I} - \mathbf{B}_C)^T (\mathbf{I} - \mathbf{B}_C) \\ &= \mathbf{O}\end{aligned}\quad (4.4.42)$$

where we have also taken into account the skew-symmetric nature of $\mathbf{B}_C$. In lossless case, $\mathbf{P}$ is a null matrix which is positive semidefinite. As from matrix norm stability analysis, since both $\mathbf{D}_A$ and $\mathbf{D}_B$ are null matrices, we find that

$$\|M_A\|_2 = 1, \quad \|M_B\|_2 = 1 \quad (4.4.43)$$

is always true. Therefore, the ADI-FDTD scheme in lossless media is unconditionally stable.

4.5 Von Neumann Method

Instead of analyzing in time domain, the Von Neumann method is often adopted for homogeneous media where all field components are transformed into Fourier domain. Doing so, (4.2.10) in Fourier domain read:

$$(\mathbf{I}_6 + \tilde{\mathbf{D}}_A - \tilde{\mathbf{D}}_C \tilde{\mathbf{A}}) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{I}_6 - \tilde{\mathbf{D}}_B + \tilde{\mathbf{D}}_C \tilde{\mathbf{B}}) \mathbf{u}^n \quad (4.5.1a)$$

$$(\mathbf{I}_6 + \tilde{\mathbf{D}}_B - \tilde{\mathbf{D}}_C \tilde{\mathbf{B}}) \mathbf{u}^{n+1} = (\mathbf{I}_6 - \tilde{\mathbf{D}}_A + \tilde{\mathbf{D}}_C \tilde{\mathbf{A}}) \mathbf{u}^{n+\frac{1}{2}}. \quad (4.5.1b)$$

where

$$\tilde{\mathbf{u}} = \begin{bmatrix} \tilde{E}_x & \tilde{E}_y & \tilde{E}_z & \tilde{H}_x & \tilde{H}_y & \tilde{H}_z \end{bmatrix}^T \quad (4.5.2)$$

$$\tilde{\mathbf{A}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -jK_y \\ 0 & 0 & 0 & -jK_z & 0 & 0 \\ 0 & 0 & 0 & 0 & -jK_x & 0 \\ 0 & -jK_z & 0 & 0 & 0 & 0 \\ 0 & 0 & -jK_x & 0 & 0 & 0 \\ -jK_y & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.5.3)$$

$$\tilde{\mathbf{B}} = \begin{bmatrix} 0 & 0 & 0 & 0 & jK_z & 0 \\ 0 & 0 & 0 & 0 & 0 & jK_x \\ 0 & 0 & 0 & jK_y & 0 & 0 \\ 0 & 0 & jK_y & 0 & 0 & 0 \\ jK_z & 0 & 0 & 0 & 0 & 0 \\ 0 & jK_x & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.5.4)$$

$$K_\xi = 2 \sin(k_\xi \Delta_\xi / 2) / \Delta_\xi. \quad (4.5.5)$$

Note that we have added tilde sign to all related matrices and vectors to indicate Fourier domain entries. Now, $\tilde{\mathbf{D}}_A$, $\tilde{\mathbf{D}}_B$ and $\tilde{\mathbf{D}}_C$ are all 6×6 diagonal matrices which comprise material parameter matrices $\tilde{\mathbf{D}}_{\epsilon\mu} = \text{diag}(\epsilon_x, \epsilon_y, \epsilon_z, \mu_x, \mu_y, \mu_z)$ and $\tilde{\mathbf{D}}_{\sigma\sigma^*} = \text{diag}(\sigma_x, \sigma_y, \sigma_z, \sigma_x^*, \sigma_y^*, \sigma_z^*)$.

The Lyapunov and matrix norm stability analysis detailed above is still applicable. This can be done by substituting all related matrices and vectors with their associated complex counterpart, and replacing all matrix and vector transpose operator with hermitian (complex). It should be pointed out that the complex matrices $\tilde{\mathbf{A}}_c = \tilde{\mathbf{D}}_C^{\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}_C^{\frac{1}{2}}$ and $\tilde{\mathbf{B}}_c = \tilde{\mathbf{D}}_C^{\frac{1}{2}} \tilde{\mathbf{B}} \tilde{\mathbf{D}}_C^{\frac{1}{2}}$ are now skew-hermitian ($\tilde{\mathbf{A}}_c = -\tilde{\mathbf{A}}_c^H$, $\tilde{\mathbf{B}}_c = -\tilde{\mathbf{B}}_c^H$). Using the same procedures in Sections 5.2 and 5.3, it can be shown in Fourier domain that averaging, forward-backward, backward-forward, ETD, forward-forward and lossless schemes are all unconditionally stable. For backward-backward scheme,

we arrive at the following mapped $\tilde{\mathbf{D}}_{m3}$ in Fourier domain from (4.4.35) as

$$\tilde{\mathbf{D}}_{m3} = \frac{\Delta t}{2} \tilde{\mathbf{D}}_{\epsilon\mu}^{-1} \tilde{\mathbf{D}}_{\sigma\sigma^*} \left(2\mathbf{I}_6 - \frac{\Delta t}{2} \tilde{\mathbf{D}}_{\epsilon\mu}^{-1} \tilde{\mathbf{D}}_{\sigma\sigma^*} \right)^{-1}. \quad (4.5.6)$$

Similar to the analysis in time domain, the positive definiteness of $\tilde{\mathbf{D}}_{m3}$ is required to ensure stability. In order for $\tilde{\mathbf{D}}_{m3}$ to be positive definite, the following condition must hold:

$$\left(2\mathbf{I}_6 - \frac{\Delta t}{2} \tilde{\mathbf{D}}_{\epsilon\mu}^{-1} \tilde{\mathbf{D}}_{\sigma\sigma^*} \right)^{-1} > 0 \quad (4.5.7)$$

Solving (4.5.7) for Δt , the condition to ensure stability for backward-backward scheme in Fourier domain is given by

$$\Delta t < 4 \left(\min_{\xi=x,y,z} \left\{ \frac{\epsilon_\xi}{\sigma_\xi}, \frac{\mu_\xi}{\sigma_\xi^*} \right\} \right) \quad (4.5.8)$$

where ϵ_ξ , σ_ξ , μ_ξ , σ_ξ^* and Δt are all positive. For inhomogeneous media, ϵ_ξ , σ_ξ , μ_ξ , σ_ξ^* are typically chosen such that $\frac{\epsilon_\xi}{\sigma_\xi}$ and $\frac{\mu_\xi}{\sigma_\xi^*}$ are the minimum among different media considered within the whole computational domain. Thus, the condition (4.5.8) in Fourier domain is similar to (4.4.37) in time domain.

4.6 Unifications of Source-Incorporated ADI-FDTD Schemes for Doubly Lossy Media

4.6.1 Unified Conventional Form (With RHS Matrix-Operators)

The previous section has discussed many possible schemes in conventional form of ADI-FDTD method for doubly lossy media, it would be desirable if all those schemes can be unified and generalized. The aforementioned schemes are first unified based on the conventional form of ADI-FDTD method as

$$(\mathbf{I}_6 - \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{D}_u + \mathbf{B}_L) \mathbf{u}^n + \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}} \quad (4.6.1a)$$

$$(\mathbf{I}_6 - \mathbf{B}_L) \mathbf{u}^{n+1} = (\mathbf{D}_u + \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} + \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}} \quad (4.6.1b)$$

where

$$\mathbf{u} = [E_x, E_y, E_z, H_x, H_y, H_z]^T \quad (4.6.2)$$

Here, we have opted the vector $\mathbf{u}$ in (4.6.2) comprising 6 fixed field components as opposed to computational domain size dependent field components in (4.2.11) for simplicity. We have also incorporated the symmetric source implementation [62–65] where $\mathbf{s}$ is the current source vector. $\mathbf{D}_u$ (diagonal), $\mathbf{A}_L$, $\mathbf{D}_s$ (diagonal) and $\mathbf{B}_L$ for various schemes are listed in Table 4.1. With such formulation, all previous schemes can be concisely described by (4.6.1) along with Table 4.1. Such unified form is amenable to the same computer code for all the schemes, except possibly with different update coefficients. All schemes are directly reducible to the lossless case when $\mathbf{L}$ is null, except for ETD scheme where $\mathbf{A}_L$, $\mathbf{B}_L$ and $\mathbf{D}_s$ are undefined. For ETD scheme, when $\mathbf{L}$ is approaching null, the expressions of $\mathbf{A}_L$, $\mathbf{B}_L$ and $\mathbf{D}_s$ can assume those of the averaging scheme because the update coefficients of the latter scheme is essentially a Pade approximation of the former scheme up to second order in time. Note however that (4.6.1) still involves matrix operators $\mathbf{A}$ and $\mathbf{B}$ (embedded in $\mathbf{A}_L$ and $\mathbf{B}_L$) at the RHS. $\mathbf{A}$ and $\mathbf{B}$ are the splitting matrix operators commonly used in ADI-FDTD compact notations [121]:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{1}{\epsilon} \partial_y \\ 0 & 0 & 0 & \frac{1}{\epsilon} \partial_z & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\epsilon} \partial_x & 0 \\ 0 & \frac{1}{\mu} \partial_z & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\mu} \partial_x & 0 & 0 & 0 \\ \frac{1}{\mu} \partial_y & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.6.3)$$

Table 4.1: Matrices for various ADI-FDTD schemes for lossy media

Scheme	$\mathbf{A}_L$	$\mathbf{B}_L$
ETD	$\mathbf{L}^{-1}(\mathbf{I}_6 - e^{-\mathbf{L}\frac{\Delta t}{2}})\mathbf{A}$	$\mathbf{L}^{-1}(\mathbf{I}_6 - e^{-\mathbf{L}\frac{\Delta t}{2}})\mathbf{B}$
Avg	$\frac{\Delta t}{2} \left(\mathbf{I}_6 + \frac{\Delta t}{4}\mathbf{L} \right)^{-1} \mathbf{A}$	$\frac{\Delta t}{2} \left(\mathbf{I}_6 + \frac{\Delta t}{4}\mathbf{L} \right)^{-1} \mathbf{B}$
F-F	$\frac{\Delta t}{2} \left(\mathbf{I}_6 + \frac{\Delta t}{2}\mathbf{L} \right)^{-1} \mathbf{A}$	$\frac{\Delta t}{2} \left(\mathbf{I}_6 + \frac{\Delta t}{2}\mathbf{L} \right)^{-1} \mathbf{B}$
F-B	$\frac{\Delta t}{2} (\mathbf{A} - \mathbf{L})$	$\frac{\Delta t}{2} \mathbf{B}$

Scheme	$\mathbf{D}_u$	$\mathbf{D}_s$
ETD	$e^{-\mathbf{L}\frac{\Delta t}{2}}$	$\mathbf{L}^{-1}(\mathbf{I}_6 - e^{-\mathbf{L}\frac{\Delta t}{2}})$
Avg	$\left(\mathbf{I}_6 + \frac{\Delta t}{4}\mathbf{L} \right)^{-1} \left(\mathbf{I}_6 - \frac{\Delta t}{4}\mathbf{L} \right)$	$\frac{\Delta t}{2} \left(\mathbf{I}_6 + \frac{\Delta t}{4}\mathbf{L} \right)^{-1}$
F-F	$\left(\mathbf{I}_6 + \frac{\Delta t}{2}\mathbf{L} \right)^{-1}$	$\frac{\Delta t}{2} \left(\mathbf{I}_6 + \frac{\Delta t}{2}\mathbf{L} \right)^{-1}$
F-B	$\mathbf{I}_6$	$\frac{\Delta t}{2}$

ETD: Exponential Time Differencing; Avg: Averaging;

F-F: Forward-Forward; F-B: Forward-Backward

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{-1}{\epsilon}\partial_z & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{-1}{\epsilon}\partial_x \\ 0 & 0 & 0 & \frac{-1}{\epsilon}\partial_y & 0 & 0 \\ 0 & 0 & \frac{-1}{\mu}\partial_y & 0 & 0 & 0 \\ \frac{-1}{\mu}\partial_z & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-1}{\mu}\partial_x & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.6.4)$$

and $\mathbf{L}$ is the diagonal loss matrix $\mathbf{L} = \text{diag} \left(\left[\frac{\sigma}{\epsilon}, \frac{\sigma}{\epsilon}, \frac{\sigma}{\epsilon}, \frac{\sigma^*}{\mu}, \frac{\sigma^*}{\mu}, \frac{\sigma^*}{\mu} \right] \right)$. Other schemes of backward-forward and backward-backward schemes are not included in the unifications because the former is essentially a dual of the forward-backward scheme, while the latter is not unconditionally stable.

4.6.2 Unified Efficient Fundamental Form (With RHS Matrix-Operator-Free)

We next proceed to transform the unified schemes (4.6.1) into efficient fundamental form of ADI-FDTD method. Introducing the (temporary) auxiliary $\hat{\mathbf{v}}$'s, (4.6.1) is rewritten as

$$\hat{\mathbf{v}}^n = (\mathbf{D}_u + \mathbf{B}_L) \mathbf{u}^n \quad (4.6.5a)$$

$$(\mathbf{I}_6 - \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^n + \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}} \quad (4.6.5b)$$

$$\hat{\mathbf{v}}^{n+\frac{1}{2}} = (\mathbf{D}_u + \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} + \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}} \quad (4.6.5c)$$

$$(\mathbf{I}_6 - \mathbf{B}_L) \mathbf{u}^{n+1} = \hat{\mathbf{v}}^{n+\frac{1}{2}}. \quad (4.6.5d)$$

Next, (4.6.5d) is expressed at one time step backward as

$$\hat{\mathbf{v}}^{n-\frac{1}{2}} = (\mathbf{I}_6 - \mathbf{B}_L) \mathbf{u}^n \quad (4.6.6)$$

and (4.6.5a) can be subsequently reduced into

$$\begin{aligned} \hat{\mathbf{v}}^n &= (\mathbf{D}_u + \mathbf{B}_L) \mathbf{u}^n \\ &= (\mathbf{I}_6 + \mathbf{D}_u) \mathbf{u}^n - (\mathbf{I}_6 - \mathbf{B}_L) \mathbf{u}^n \\ &= (\mathbf{I}_6 + \mathbf{D}_u) \mathbf{u}^n - \hat{\mathbf{v}}^{n-\frac{1}{2}}. \end{aligned} \quad (4.6.7)$$

Similarly, by rewriting (4.6.5b) as

$$\hat{\mathbf{v}}^n = (\mathbf{I}_6 - \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} - \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}}, \quad (4.6.8)$$

(4.6.5c) is reducible to

$$\begin{aligned} \hat{\mathbf{v}}^{n+\frac{1}{2}} &= (\mathbf{D}_u + \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} + \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}} \\ &= (\mathbf{I}_6 + \mathbf{D}_u) \mathbf{u}^{n+\frac{1}{2}} - [(\mathbf{I}_6 - \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} - \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}}] \\ &= (\mathbf{I}_6 + \mathbf{D}_u) \mathbf{u}^{n+\frac{1}{2}} - \hat{\mathbf{v}}^n \end{aligned} \quad (4.6.9)$$

Finally, the unified schemes in efficient fundamental form of ADI-FDTD method read:

$$\hat{\mathbf{v}}^n = (\mathbf{I}_6 + \mathbf{D}_u) \mathbf{u}^n - \hat{\mathbf{v}}^{n-\frac{1}{2}} \quad (4.6.10a)$$

$$(\mathbf{I}_6 - \mathbf{A}_L) \mathbf{u}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^n + \mathbf{D}_s \mathbf{s}^{n+\frac{1}{2}} \quad (4.6.10b)$$

$$\hat{\mathbf{v}}^{n+\frac{1}{2}} = (\mathbf{I}_6 + \mathbf{D}_u) \mathbf{u}^{n+\frac{1}{2}} - \hat{\mathbf{v}}^n \quad (4.6.10c)$$

$$(\mathbf{I}_6 - \mathbf{B}_L) \mathbf{u}^{n+1} = \hat{\mathbf{v}}^{n+\frac{1}{2}} \quad (4.6.10d)$$

with initialization $\hat{\mathbf{v}}^{-\frac{1}{2}} = (\mathbf{I}_6 - \mathbf{B}_L) \mathbf{u}^0$. Now, (4.6.10a)-(4.6.10b) forms the first substep while (4.6.10c)-(4.6.10d) forms the second. Note that (4.6.10) has been formulated in the simplest, most concise, most efficient, and most fundamental form of ADI-FDTD scheme with its RHS free of matrix operators $\mathbf{A}$ and $\mathbf{B}$ (It is the simplest because there are no more $\mathbf{A}$ and $\mathbf{B}$ to be simplified further at RHS). Besides, the source is incorporated concisely at only the first substep (4.6.10a)-(4.6.10b) in the unified efficient FADI-FDTD schemes.

4.7 Implementation of Unified Efficient FADI-FDTD Schemes

4.7.1 Unified Update Equations

We now provide the update equations for (4.6.10). Assuming only electric current density, J , and defining

$$\mathbf{u} = [E_x, E_y, E_z, H_x, H_y, H_z]^T \quad (4.7.1)$$

$$\hat{\mathbf{v}} = [\hat{e}_x, \hat{e}_y, \hat{e}_z, \hat{h}_x, \hat{h}_y, \hat{h}_z]^T \quad (4.7.2)$$

$$\mathbf{s} = \left[\frac{-1}{\epsilon} J_x, \frac{-1}{\epsilon} J_y, \frac{-1}{\epsilon} J_z, 0, 0, 0 \right]^T, \quad (4.7.3)$$

the unified update equations of efficient FADI-FDTD schemes read

First substep from n to $n + \frac{1}{2}$:

1) Auxiliary (explicit) update for $\hat{e}$ and $\hat{h}$

$$\hat{e}_x|_{i+\frac{1}{2},j,k}^n = c_{ea}E_x|_{i+\frac{1}{2},j,k}^n - \hat{e}_x|_{i+\frac{1}{2},j,k}^{n-\frac{1}{2}} \quad (4.7.4a)$$

$$\hat{e}_y|_{i,j+\frac{1}{2},k}^n = c_{ea}E_y|_{i,j+\frac{1}{2},k}^n - \hat{e}_y|_{i,j+\frac{1}{2},k}^{n-\frac{1}{2}} \quad (4.7.4b)$$

$$\hat{e}_z|_{i,j,k+\frac{1}{2}}^n = c_{ea}E_z|_{i,j,k+\frac{1}{2}}^n - \hat{e}_z|_{i,j,k+\frac{1}{2}}^{n-\frac{1}{2}} \quad (4.7.4c)$$

$$\hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n = c_{ha}H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n - \hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n-\frac{1}{2}} \quad (4.7.4d)$$

$$\hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n = c_{ha}H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n - \hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n-\frac{1}{2}} \quad (4.7.4e)$$

$$\hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n = c_{ha}H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n - \hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n-\frac{1}{2}} \quad (4.7.4f)$$

2) Implicit update for E

$$\begin{aligned} & \left(1 + \frac{bd}{\Delta y^2} + \frac{bd_-}{\Delta y^2}\right) E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} - \frac{bd}{\Delta y^2} E_x|_{i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - \frac{bd_-}{\Delta y^2} E_x|_{i+\frac{1}{2},j-1,k}^{n+\frac{1}{2}} \\ &= c_{e1}\hat{e}_x|_{i+\frac{1}{2},j,k}^n + \frac{c_{e2}}{\Delta y} \hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n - \frac{c_{e3}}{\Delta y} \hat{h}_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^n - c_{e4}J_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} \end{aligned} \quad (4.7.5a)$$

$$\begin{aligned} & \left(1 + \frac{bd}{\Delta z^2} + \frac{bd_-}{\Delta z^2}\right) E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} - \frac{bd}{\Delta z^2} E_y|_{i,j+\frac{1}{2},k+1}^{n+\frac{1}{2}} - \frac{bd_-}{\Delta z^2} E_y|_{i,j+\frac{1}{2},k-1}^{n+\frac{1}{2}} \\ &= c_{e1}\hat{e}_y|_{i,j+\frac{1}{2},k}^n + \frac{c_{e2}}{\Delta z} \hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n - \frac{c_{e3}}{\Delta z} \hat{h}_x|_{i,j+\frac{1}{2},k-\frac{1}{2}}^n - c_{e4}J_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} \end{aligned} \quad (4.7.5b)$$

$$\begin{aligned} & \left(1 + \frac{bd}{\Delta x^2} + \frac{bd_-}{\Delta x^2}\right) E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \frac{bd}{\Delta x^2} E_z|_{i+1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \frac{bd_-}{\Delta x^2} E_z|_{i-1,j,k+\frac{1}{2}}^{n+\frac{1}{2}} \\ &= c_{e1}\hat{e}_z|_{i,j,k+\frac{1}{2}}^n + \frac{c_{e2}}{\Delta x} \hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n - \frac{c_{e3}}{\Delta x} \hat{h}_y|_{i-\frac{1}{2},j,k+\frac{1}{2}}^n - c_{e4}J_z|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} \end{aligned} \quad (4.7.5c)$$

3) Explicit update for H

$$H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} = c_{h1}\hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n + \frac{c_{h2}}{\Delta z} \left(E_y|_{i,j+\frac{1}{2},k+1}^n - E_y|_{i,j+\frac{1}{2},k}^n\right) \quad (4.7.6a)$$

$$H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} = c_{h1}\hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n + \frac{c_{h2}}{\Delta x} \left(E_z|_{i+1,j,k+\frac{1}{2}}^n - E_z|_{i,j,k+\frac{1}{2}}^n\right) \quad (4.7.6b)$$

$$H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} = c_{h1}\hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n + \frac{c_{h2}}{\Delta y} \left(E_x|_{i+\frac{1}{2},j+1,k}^n - E_x|_{i+\frac{1}{2},j,k}^n\right) \quad (4.7.6c)$$

Second substep from $n + \frac{1}{2}$ to $n + 1$:

1) Auxiliary (explicit) update for $\hat{e}$ and $\hat{h}$

$$\hat{e}_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} = c_{ea}E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} - \hat{e}_x|_{i+\frac{1}{2},j,k}^n \quad (4.7.7a)$$

$$\hat{e}_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} = c_{ea}E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} - \hat{e}_y|_{i,j+\frac{1}{2},k}^n \quad (4.7.7b)$$

$$\hat{e}_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} = c_{ea}E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{e}_z|_{i,j,k+\frac{1}{2}}^n \quad (4.7.7c)$$

$$\hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} = c_{ha}H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n \quad (4.7.7d)$$

$$\hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} = c_{ha}H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n \quad (4.7.7e)$$

$$\hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} = c_{ha}H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - \hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n \quad (4.7.7f)$$

2) Implicit update for E

$$\begin{aligned} & \left(1 + \frac{bd}{\Delta z^2} + \frac{bd_-}{\Delta z^2}\right) E_x|_{i+\frac{1}{2},j,k}^{n+1} - \frac{bd}{\Delta z^2} E_x|_{i+\frac{1}{2},j,k+1}^{n+1} - \frac{bd_-}{\Delta z^2} E_x|_{i+\frac{1}{2},j,k-1}^{n+1} \\ &= c_{e1}\hat{e}_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} + \frac{c_{e2}}{\Delta z}\hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \frac{c_{e3}}{\Delta z}\hat{h}_y|_{i+\frac{1}{2},j,k-\frac{1}{2}}^{n+\frac{1}{2}} \end{aligned} \quad (4.7.8a)$$

$$\begin{aligned} & \left(1 + \frac{bd}{\Delta x^2} + \frac{bd_-}{\Delta x^2}\right) E_y|_{i,j+\frac{1}{2},k}^{n+1} - \frac{bd}{\Delta x^2} E_y|_{i+1,j+\frac{1}{2},k}^{n+1} - \frac{bd_-}{\Delta x^2} E_y|_{i-1,j+\frac{1}{2},k}^{n+1} \\ &= c_{e1}\hat{e}_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} + \frac{c_{e2}}{\Delta x}\hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} - \frac{c_{e3}}{\Delta x}\hat{h}_z|_{i-\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} \end{aligned} \quad (4.7.8b)$$

$$\begin{aligned} & \left(1 + \frac{bd}{\Delta y^2} + \frac{bd_-}{\Delta y^2}\right) E_z|_{i,j,k+\frac{1}{2}}^{n+1} - \frac{bd}{\Delta y^2} E_z|_{i,j+1,k+\frac{1}{2}}^{n+1} - \frac{bd_-}{\Delta y^2} E_z|_{i,j-1,k+\frac{1}{2}}^{n+1} \\ &= c_{e1}\hat{e}_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{c_{e2}}{\Delta y}\hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - \frac{c_{e3}}{\Delta y}\hat{h}_x|_{i,j-\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} \end{aligned} \quad (4.7.8c)$$

3) Explicit update for H

$$H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} = c_{h1}\hat{h}_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{c_{h2}}{\Delta y} \left(E_z|_{i,j+1,k+\frac{1}{2}}^{n+\frac{1}{2}} - E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} \right) \quad (4.7.9a)$$

$$H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+1} = c_{h1}\hat{h}_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{c_{h2}}{\Delta z} \left(E_x|_{i+\frac{1}{2},j,k+1}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} \right) \quad (4.7.9b)$$

$$H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = c_{h1}\hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} + \frac{c_{h2}}{\Delta x} \left(E_y|_{i+1,j+\frac{1}{2},k}^{n+\frac{1}{2}} - E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} \right) \quad (4.7.9c)$$

All the update coefficients and associated parameters for various schemes are tabulated in Table 4.2. Note that for simplicity, we have omitted the subscript indices for all media parameters ϵ , σ , μ , σ^* and b , d , p , q . In fact, the subscript indices of ϵ , σ , b

Table 4.2: Coefficients and parameters of update equations for various efficient FADI-FDTD schemes

Scheme	Implicit Update				Explicit Update			
	c_{e1}	c_{e2}	c_{e3}	c_{e4}	c_{h1}	c_{h2}	c_{ea}	c_{ha}
ETD	1	b	b	b	1	d	$1 + p$	$1 + q$
Avg	1	b	b	b	1	d	p	q
F-F	1	b	b	b	1	d	$1 + p$	$1 + q$
F-B	p	bq	bq_-	b	$2q$	d	2	2

Scheme	b	d	p	q
ETD	$\frac{1-e^{-\Delta t\sigma/2\epsilon}}{\sigma}$	$\frac{1-e^{-\Delta t\sigma^*/2\mu}}{\sigma^*}$	$e^{-\Delta t\sigma/2\epsilon}$	$e^{-\Delta t\sigma^*/2\mu}$
Avg	$\frac{\Delta t/2\epsilon}{(1+\frac{\Delta t\sigma}{4\epsilon})}$	$\frac{\Delta t/2\mu}{(1+\frac{\Delta t\sigma^*}{4\mu})}$	$\frac{2}{(1+\frac{\Delta t\sigma}{4\epsilon})}$	$\frac{2}{(1+\frac{\Delta t\sigma^*}{4\mu})}$
F-F	$\frac{\Delta t/2\epsilon}{(1+\frac{\Delta t\sigma}{2\epsilon})}$	$\frac{\Delta t/2\mu}{(1+\frac{\Delta t\sigma^*}{2\mu})}$	$\frac{1}{(1+\frac{\Delta t\sigma}{2\epsilon})}$	$\frac{1}{(1+\frac{\Delta t\sigma^*}{2\mu})}$
F-B	$\frac{\Delta t/2\epsilon}{(1+\frac{\Delta t\sigma}{2\epsilon})}$	$\frac{\Delta t/2\mu}{(1+\frac{\Delta t\sigma^*}{2\mu})}$	$\frac{1}{(1+\frac{\Delta t\sigma}{2\epsilon})}$	$\frac{1}{(1+\frac{\Delta t\sigma^*}{2\mu})}$

and p should follow that of the electric fields, whereas those of μ , σ^* , d and q follow that of the magnetic fields. For instance, in (4.7.4a), (4.7.4f), (4.7.5a), (4.7.6c), b and p have subscript indices of $i + \frac{1}{2}, j, k$ while d and q have those of $i + \frac{1}{2}, j + \frac{1}{2}, k$. For d_- and q_- , the subscript indices are $i + \frac{1}{2}, j - \frac{1}{2}, k$ where $d_- = d_{i+\frac{1}{2}, j-\frac{1}{2}, k}$ and $q_- = q_{i+\frac{1}{2}, j-\frac{1}{2}, k}$. It should be reminded that no electric current source J is needed in the second substep, which is made possible by the efficient fundamental form (4.6.10c)-(4.6.10d). For forward-backward scheme, the update coefficients in the second substep are derived by setting σ and σ^* equal zero (lossless) [53].

Examining (4.7.5) indicates that the number of RHS update coefficients and field variables are substantially lower than that of the conventional ADI-FDTD schemes (Eq. (11) in [47]). Moreover, a look at Table 4.2 reveals that the update coefficients c_{e2} , c_{e3} and c_{e4} are the same (independent of μ and σ^*) for ETD, averaging and forward-forward schemes. This is particularly useful for inhomogeneous mag-

Table 4.3: Comparisons of number of arithmetic operations per grid between conventional and efficient fundamental forms of ADI-FDTD schemes for lossy media over one complete time step

Arithmetic operations		Conventional form	Efficient fundamental form
Implicit, RHS	M/D	84	12
	A/S	48	12
Explicit, RHS	M/D	30	30
	A/S	24	24
Total, RHS	M/D	114	42
	A/S	72	36
	M/D + A/S	186	78
Tridiag. matrices inversion	M/D	18	18
	A/S	12	12
Overall	M/D	132	60
	A/S	84	48
	M/D + A/S	216	108
Efficiency gain	RHS	1	2.38
	Overall	1	2

netic media where no additional memory indexing is required in the electric field update equations (4.7.5). For forward-backward scheme, the simplicity lies in the second substep where the algorithm is as easy as implementing a lossless ADI-FDTD method. Lastly, the symmetric current source excitation [62–65] is only needed in the first substep for all efficient fundamental schemes. All the aforementioned advantages contribute towards reducing the flops count and memory indexing throughout the whole update procedures and thus improving the overall efficiency compared to the conventional ADI-FDTD schemes.

Table 4.3 shows the comparisons of number of arithmetic operations per grid between

conventional and efficient fundamental forms of ADI-FDTD schemes for lossy media over one complete time step. The number of multiplications/divisions (M/D) and additions/subtractions (A/S) are determined from (4.6.1a)-(4.6.1b) for conventional form of ADI-FDTD and (4.6.10a)-(4.6.10d) for efficient fundamental form of ADI-FDTD. We can see that the total flops count for the RHS is considerably less for the efficient fundamental form (78 against 186 for conventional form), which gives an efficiency gain of 2.38. Since there is cost for solving tridiagonal systems, Table 4.3 also includes the arithmetic operations needed for inverting tridiagonal matrices. The algorithm used for the tridiagonal matrices inversion is Thomas algorithm, which is a special type of Gaussian elimination method. Taking this cost into account, the efficient fundamental form still achieves an overall efficiency gain of 2.

4.7.2 Field Memory Arrays

The field memory arrays needed for efficient FADI-FDTD schemes are initially found to be ($\xi = x, y, z$)

$$\begin{aligned} & \left\{ \hat{e}_{\xi}^{n-\frac{1}{2}}, \hat{e}_{\xi}^n, \hat{e}_{\xi}^{n+\frac{1}{2}} \right\}; \left\{ E_{\xi}^n, E_{\xi}^{n+\frac{1}{2}}, E_{\xi}^{n+1} \right\}; \\ & \left\{ \hat{h}_{\xi}^{n-\frac{1}{2}}, \hat{h}_{\xi}^n, \hat{h}_{\xi}^{n+\frac{1}{2}} \right\}; \left\{ H_{\xi}^n, H_{\xi}^{n+\frac{1}{2}}, H_{\xi}^{n+1} \right\} \end{aligned} \quad (4.7.10)$$

where the variables grouped within the same curly braces share the same memory arrays, i.e. in computer programs, they share the same variable names to be assigned with new values successively. For instance, $\left\{ \hat{e}_{\xi}^{n-\frac{1}{2}}, \hat{e}_{\xi}^n, \hat{e}_{\xi}^{n+\frac{1}{2}} \right\}$ consume 1 field memory array and the same holds for $\left\{ E_{\xi}^n, E_{\xi}^{n+\frac{1}{2}}, E_{\xi}^{n+1} \right\}$, $\left\{ \hat{h}_{\xi}^{n-\frac{1}{2}}, \hat{h}_{\xi}^n, \hat{h}_{\xi}^{n+\frac{1}{2}} \right\}$ and $\left\{ H_{\xi}^n, H_{\xi}^{n+\frac{1}{2}}, H_{\xi}^{n+1} \right\}$. Since there are x, y and z -directed fields ($\xi = x, y, z$), the total number of field memory arrays needed are $4 \times 3 = 12$.

To reduce the field memory storage, one can combine (4.7.6c) with (4.7.7c) to yield

$$\begin{aligned} \hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+\frac{1}{2}} &= (c_{ha}c_{h1} - 1)\hat{h}_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n \\ &+ \frac{c_{ha}c_{h2}}{\Delta y} \left(E_x|_{i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} \right). \end{aligned} \quad (4.7.11)$$

This can always be done because we are not interested in the intermediate magnetic field values at $n + \frac{1}{2}$. In this case, the explicit update of (4.7.6) is no longer needed and the efficiency can be further improved. Furthermore, if the final magnetic field values are not frequently needed, we can repeat the above procedures for the final magnetic field update equations in the second substep. In doing so, the field memory arrays needed are now

$$\left\{ \hat{e}_\xi^{n-\frac{1}{2}}, \hat{e}_\xi^n, \hat{e}_\xi^{n+\frac{1}{2}} \right\}; \left\{ E_\xi^n, E_\xi^{n+\frac{1}{2}}, E_\xi^{n+1} \right\}; \left\{ \hat{h}_\xi^{n-\frac{1}{2}}, \hat{h}_\xi^n, \hat{h}_\xi^{n+\frac{1}{2}} \right\}. \quad (4.7.12)$$

Now the total number of field memory arrays needed is $3 \times 3 = 9$.

For comparison, we note that in conventional ADI-FDTD schemes, the field memory arrays are given as

$$\left\{ E_\xi^n, E_\xi^{n+1} \right\}; \left\{ E_\xi^{n+\frac{1}{2}} \right\}; \left\{ H_\xi^n, H_\xi^{n+\frac{1}{2}}, H_\xi^{n+1} \right\}. \quad (4.7.13)$$

The total number of field memory arrays needed is also $3 \times 3 = 9$, which is the same as the efficient FADI-FDTD schemes.

4.7.3 Parameter Memory Arrays

Conventionally, all coefficients in Table 4.2 are computed in run time during each iteration from four media parameter memory arrays, which comprise

$$\{\epsilon\}; \{\mu\}; \{\sigma\}; \{\sigma^*\}. \quad (4.7.14)$$

To further improve the efficiency, instead of storing (4.7.14), we can first precompute

and store the following four alternative parameter memory arrays:

$$\{b\}; \{d\}; \{p\}; \{q\}. \quad (4.7.15)$$

It can be seen from Table 4.2 that, with the above alternative parameter memory arrays, all the respective RHS coefficients can be directly computed. This not only reduces the memory indexing effort but also reduces the arithmetic operations needed. For instance, with the alternative parameter memory arrays, to compute c_{e2} for ETD, averaging and forward-forward schemes, one would only need to access b instead of both ϵ and σ . No further arithmetic operations are needed. Note that such redefinition and storing of alternative parameter memory arrays is not effectively applicable in forward-backward scheme. This is because unlike the other schemes, the update coefficients of forward-backward scheme are different in both substeps (lossless in second substep).

4.7.4 PEC and PMC Implementations

Recently, PEC condition implementation within a computation domain for ADI-FDTD method has been considered in [122] by means of a modified tridiagonal matrix. Although it provides sufficient accuracy, the implementation is rather cumbersome, especially when the intended PEC structure is of arbitrary shape and not planar in nature. In this subsection, we make use of our efficient FADI-FDTD schemes for lossy media to implement PEC or PMC conveniently inside a computation domain. This can be directly realized by taking the limit of all the update coefficients tabulated in Table 4.2 when σ or σ^* tends to infinity. Note that such limit exists for all efficient FADI-FDTD schemes. Although the update procedures of the conventional ADI-FDTD schemes are not shown explicitly, it should be pointed out that for its forward-backward scheme, some RHS update coefficients of second substep will be undefined when σ or σ^* tends to infinity. Therefore, the implementa-

tion of PEC or PMC will fail in the forward-backward scheme in conventional form of ADI-FDTD method, but not in the forward-backward scheme in our efficient FADI-FDTD method.

4.8 Numerical Results

4.8.1 CPU Time Saving

In this subsection, we compute the CPU time needed to run using various schemes of ADI-FDTD for lossy media in a PEC cavity of $50 \times 50 \times 51$ cells. The programs have been compiled using Microsoft Visual C++ under Microsoft Windows XP operating system (OS), and run on a platform of 2.66 GHz Intel Duo Core Processor with 4 GB RAM. We consider the alternative parameter memory arrays given in (4.7.15), i.e. all the respective RHS coefficients are directly computed, to reduce all the memory indexing effort and arithmetic operations. ϵ , μ , σ and σ^* can be of arbitrary values at different grid points. Cell size is set at 50 mm and Δt is specified at CFLN=5 where $\text{CFLN} = \Delta t / \Delta t_{\text{CFL}}$, and Δt_{CFL} is the CFL limit in Yee's explicit FDTD method. A z -directed monochromatic sinusoidal point current source with frequency 300 MHz is excited at the centre (i_s, j_s, k_s) of the cavity. The program is run for a total of 100 time steps.

Table 4.4 shows the relative CPU time incurred for various ADI-FDTD schemes for lossy media, with respect to the reference Yee's explicit FDTD method [2]. The forward-backward scheme is omitted because the storing of alternative parameter memory arrays of (4.7.15) is not effectively applicable as mentioned earlier. Note that the time step used in the reference Yee's explicit FDTD method is set at its maximum allowed limit of CFLN=1 to ensure stability. All ADI-FDTD schemes incurs the same relative CPU time due to the fact that all RHS coefficients are

precomputed. At CFLN=5, the conventional form of ADI-FDTD schemes incur relative CPU time of 0.83 while the efficient fundamental form of ADI-FDTD schemes incur relative CPU time of 0.33. With the aforementioned advantages of the efficient fundamental form of ADI-FDTD schemes (such as reduced RHS coefficients, field variables, etc.), the efficiency gain over the conventional form of ADI-FDTD schemes is around 2.5. Moreover, if compared against the Yee's explicit FDTD method, the efficiency gain is further increased to 3. This makes our efficient fundamental form of ADI-FDTD schemes attractive for its high algorithm efficiency. The RAM needed for efficient fundamental form of ADI-FDTD schemes is the same as the conventional form counterpart but higher than the Yee's explicit FDTD due to additional field memory arrays.

Table 4.5 further shows the efficiency gain in terms of CPU time achieved by efficient fundamental form over conventional form of ADI-FDTD and Yee's explicit FDTD for different computational domain sizes. For $50 \times 50 \times 50$ and $100 \times 100 \times 100$ computational domain sizes, the efficiency gain over the conventional form of ADI-FDTD is around 2 to 2.5 while the efficiency gain over the Yee's explicit FDTD is 3. For large computational domain size of $250 \times 250 \times 250$, the efficient fundamental form of ADI-FDTD still achieves an efficiency gain of 1.3 and 2 over conventional ADI-FDTD and Yee's explicit FDTD, respectively. The lower efficiency gain in large computational domain size may be attributed to the bottleneck caused by the memory indexing, where its computational cost is more expensive than the computational cost of arithmetic operations.

4.8.2 Numerical Examples for PEC and PMC Implementations

The implementation of PEC and PMC can also be used as a gauge for accuracy assessment for the efficient FADI-FDTD schemes detailed. For this purpose, we

Table 4.4: Relative CPU time for various ADI-FDTD schemes for lossy media

ADI-FDTD	Relative CPU time		
	Avg	ETD	F-F
Conventional form	0.83	0.83	0.83
Efficient fundamental form	0.33	0.33	0.33

Efficiency gain over conventional ADI-FDTD	2.5	2.5	2.5
Efficiency gain over explicit FDTD	3.0	3.0	3.0

Table 4.5: Efficiency gain in terms of CPU time achieved by efficient fundamental form over conventional form of ADI-FDTD and explicit FDTD for different computational domain sizes

Domain size	Efficiency gain	
	over conventional ADI-FDTD	explicit FDTD
$50 \times 50 \times 50$	2.5	3.0
$100 \times 100 \times 100$	2.1	3.0
$250 \times 250 \times 250$	1.3	2.0

consider a $50 \times 50 \times 50$ cells cavity of uniform cell size 3 mm with a PEC sphere located at the centre and the rest free space. The radius of the PEC sphere is 30 mm. The PEC medium is realized by setting σ to the extreme value of 10^{308} . A z -directed line current source of modulated Gaussian pulse with centre frequency 5 GHz extending from top to bottom of the cavity is located 24 mm away from the PEC sphere. The source illuminates upon the PEC sphere and the electric field leakage is measured at the centre of the PEC sphere throughout 1000 time steps with CFLN equals 5. The numerical experiments are carried out using different efficient FADI-FDTD schemes detailed. The PEC sphere is then replaced by a PMC sphere by setting σ^* to 10^{308} instead of σ , and the electric field leakage is also measured at

Figure 4.1: Normalized electric field leakage recorded at the centre of PEC sphere using different schemes. Only forward-backward scheme exhibits electric field leakage.

the centre of the PMC sphere.

Fig. 4.1 and Fig. 4.2 show the electric field leakage recorded at centre of PEC and PMC spheres normalized to the maximum value of electric field at the exterior. Analytically, no fields shall be able to penetrate the PEC or PMC material. We note that all three averaging, ETD and forward-forward schemes record zero electric field at the centre of the PEC and PMC spheres. On the contrary, forward-backward scheme records a field leakage of around 0.1 percent, which indicates the inaccuracy of the scheme.

4.8.3 Asymmetry and Numerical Errors

Next, we proceed to analyze the asymmetry and numerical errors posed by various ADI-FDTD schemes for lossy media. Comparisons of these errors could be made with either conventional or efficient fundamental form since both forms can be transformed into each other (and essentially yield the same computation). We adopt a dimension of $20 \times 20 \times 21$ cells, $\epsilon = \epsilon_0$, $\mu = \mu_0$, $\sigma = 10^{-4}$ S/m and $\sigma^* = 0.05$ Ω /m.

Figure 4.2: Same as Fig. 4.1, but for PMC sphere. Again, only forward-forward scheme exhibits electric field leakage.

Cell size, Δt and source are the same as the previous subsection. We also define the electric field asymmetry error as

$$E_{asymerr} = 20 \log \frac{|E_{z(i,j,ks)} - E_{z(j,i,ks)}|}{\max(|E_z|)} \quad (4.8.1)$$

Fig. 4.3 shows the the asymmetry error (in dB) with respect to x and y grid positions for various ADI-FDTD schemes. It can be seen that averaging, ETD and forward-forward schemes have very low level of electric field asymmetry error (in the vicinity of -320 dB). On the other hand, even though symmetric source is implemented, forward-backward scheme still records considerably higher electric field asymmetry error. We hereby point out that the symmetric source implementation described in [62–65] also utilized forward-backward scheme for its independent current source J , i.e. J is forward (at $n + \frac{1}{2}$) in the first substep and backward (still at $n + \frac{1}{2}$) in the second. While it was shown previously that the forward-backward scheme of an *independent* source is accurate and has lower electric field asymmetry error, similar argument cannot be applied here if the source is *dependent* on electric field, such as in the case of lossy media here, where $J = \sigma E$.

Figure 4.3: Asymmetry error (in dB) with respect to x and y grid positions for (a) exponential time differencing, (b) averaging, (c) forward-forward and (d) forward-backward schemes. Forward-backward scheme records considerably higher electric field asymmetry error.

To further compare the accuracy among ETD, averaging and forward-forward schemes, we now consider $20 \times 20 \times 21$ cells cavity of doubly lossy media with $\sigma = 0.3$ S/m and $\sigma^* = 60$ Ω /m. A z -directed line current source with modulated gaussian pulse excitation of centre frequency 300 MHz and bandwidth 600 MHz is flowing from bottom to top through the cavity centre. Cell size is now chosen as 16 mm to resolve $1/20$ times of the medium wavelength. Simulation is terminated after 200 and 100 time steps with CFLN equals 5 and 10, respectively. The experiment is also run using Yee's explicit FDTD method of time-averaging scheme [2], with Δt set at the CFL limit to serve as the reference. We define the normalized electric field error as

$$E_{err} = \frac{E_{FADI} - E_{explicit}}{\max(|E_{explicit}|)} \quad (4.8.2)$$

where E_{FADI} is the electric field recorded by various efficient fundamental form of ADI-FDTD schemes and $E_{explicit}$ is the electric field recorded by the Yee's explicit FDTD method. Fig. 4.4 shows the normalized electric field error recorded at position (17,17,17) using various schemes at (a) CFLN=5 and (b) CFLN=10,

Figure 4.4: Normalized electric field error exhibited by various schemes for (a) CFLN=5 and (b) CFLN=10.

respectively. The normalized error shown by ETD scheme is the lowest among all, followed by averaging, forward-forward and lastly forward-backward schemes. Note that although forward-forward scheme is only first-order accurate in time, the overall accuracy is higher than that of forward-backward scheme, which may be due to the higher asymmetry error exhibited by the latter. The highest accuracy of ETD scheme may be attributed to its closer resemblance of solution to the first-order differential equation.

Table 4.6 further shows the efficiency gain and relative root-mean-square (RMS) error of efficient FADI-FDTD schemes for various CFLNs. The efficiency gain is taken over the Yee's explicit FDTD and the RMS error is taken relative to the Yee's explicit FDTD within the whole computational domain for a sinusoidal excitation of 300 MHz. CPW is set as 20 which corresponds to cell size of 16 mm. This table gives a clear illustration on the trade-off between accuracy and efficiency of our efficient FADI-FDTD schemes. For practical CFLN of 4, the efficiency gain is 2.4, and the relative RMS error of all schemes ranges only from 4-6 percent. Even at CFLN=10, our ETD scheme consumes 6 times less simulation time than the Yee's

Table 4.6: Efficiency gain and relative root-mean-square error of efficient FADI-FDTD schemes for various CFLNs

CFLN		2	4	6	8	10
Efficiency gain		1.2	2.4	3.6	4.8	6.0
Relative RMS error	ETD	1.57%	4.38%	6.84%	8.96%	11.02%
	Avg	1.95%	6.32%	11.44%	16.18%	19.84%
	F-F	2.56%	4.83%	7.38%	10.08%	12.93%

Figure 4.5: Magnitude of reflection coefficient for a half space lossy medium computed using various schemes.

explicit FDTD, at the expense of only 11 percent relative RMS error. This implies that our efficient fundamental form of ADI-FDTD schemes achieves a good trade-off between efficiency and accuracy.

Finally, we compute the reflection coefficients of a half space lossy medium numerically. σ and σ^* of the lossy medium is set as 5 S/m and 60 Ω /m respectively. A modulated Gaussian pulse with a bandwidth of 6 GHz around centre frequency of 5 GHz is launched from the free space. Cell size is set at 0.9375 mm which corresponds to CPW of around 20 for the lossy medium at 5 GHz and CFLN=4. The reflection coefficients in frequency domain can be obtained numerically by taking the ratio of the discrete Fourier transform of the reflected wave to the discrete Fourier transform

Table 4.7: Relative permittivity, ϵ_r and conductivity, σ of skin layers at 42.25 GHz and 61.22 GHz

Skin layers	ϵ_r		σ	
	42.25 GHz	61.22 GHz	42.25 GHz	61.22 GHz
epidermis and dermis	11.40	8.00	33.00	37.40
fat	3.37	3.12	2.28	2.83

of the incident wave. Fig. 4.5 plots the magnitude of reflection coefficient for a half space lossy medium computed using various schemes and they are compared against the reference analytical reflections coefficient Γ given as

$$\Gamma = \frac{\eta_2 - \eta_1}{\eta_1 + \eta_2} \quad (4.8.3)$$

where η_1 is the wave impedance of free space at 377 Ω and η_2 is the wave impedance of the lossy medium. It is evident that the magnitude of reflection coefficient computed using ETD scheme is the closest to the magnitude of reference analytical reflection coefficient. This again shows the highest accuracy of ETD scheme among all other schemes.

4.8.4 Specific Absorption Rate (SAR)

SAR is a measure of energy absorption rate for biological media exposed to electromagnetic radiation. It can be computed from

$$SAR = \frac{1}{2} \frac{\sigma |\tilde{\mathbf{E}}|^2}{\rho} \quad (4.8.4)$$

where $\tilde{\mathbf{E}}$ is the Fourier transform of the recorded electric field components and ρ is the density of the biological media in kg/m³. The SAR has the overall unit of W/kg.

In this numerical example, the exposure of human skin to electromagnetic radiation

is considered. The human skin has a cross sectional area of $3.75 \text{ mm} \times 3.75 \text{ mm}$ in y and z directions and a depth of 2 mm in x direction. In x direction, the skin has two layers. The top layer consists of epidermis and dermis which has a total thickness of 1.5 mm , and the bottom layer consists of fat. The interaction of human skin with electromagnetic waves at two therapeutic frequencies of 42.25 GHz and 61.22 GHz are considered [123]. The relative permittivity, ϵ_r and conductivity, σ of the skin layers at these two frequencies are listed in Table 4.7 [124]. The cell size $\Delta x = \Delta y = \Delta z = \Delta$ is chosen at $75 \text{ }\mu\text{m}$ and a z -directed line current source located 1.5 mm away from the surface of the human skin illuminates upon it. The computational domain size is $50 \times 50 \times 50$ and 10 layers of PML [125] terminates the computational boundaries. The exterior boundaries of the PML is simply terminated with PEC. The perfectly matched layer used is the complex frequency shifted convolutional perfectly matched layer (CFS-CPML) having constitutive parameters

$$\sigma(\zeta) = \frac{\sigma_{max} |\zeta - \zeta_0|^m}{\delta^m} \quad (4.8.5)$$

$$\kappa(\zeta) = 1 + (\kappa_{max} - 1) \frac{|\zeta - \zeta_0|^m}{\delta^m} \quad (4.8.6)$$

where δ is the thickness of the PML, ζ_0 is the interface to free space and m is the order of the polynomial. In our simulation, $m = 4$, $\kappa_{max} = 15$ and another constitutive parameter, α is set as a constant 0.08 . σ_{max} that will minimize reflection is given as

$$\sigma_{max} = \frac{m+1}{150\pi\Delta} = 141.49 \text{ S/m}. \quad (4.8.7)$$

The SAR of human skin at 42.25 GHz and 61.22 GHz is computed using (4.8.4) at steady state. The densities of the top layer (epidermis and dermis) and bottom layer (fat) are assumed as 1000 kg/m^3 and 850 kg/m^3 , respectively. Figs. 4.6 and 4.7 plot the SAR of human skin at 42.25 GHz and 61.22 GHz , respectively. Both figures show the SAR at z cut plane of 2 mm . The SAR values at each location have been scaled to correspond to incident power density $S = \frac{1}{2} \text{Re}(\tilde{\mathbf{E}} \times \tilde{\mathbf{H}}^*)$ of 1 mW/m^2 in free

Figure 4.6: SAR of human skin at 42.25 GHz with respect to depth and width.

Figure 4.7: SAR of human skin at 61.22 GHz with respect to depth and width.

space. The SAR is computed using the efficient fundamental form of ADI-FDTD method with ETD scheme at CFLN=5. It can be seen that at 61.22 GHz, the maximum SAR at the surface of the human skin is higher than that of 42.25 GHz and the SAR quickly decreases with respect to the depth (x axis) of human skin. Fig. 4.8 further plots the SAR of human skin at $y = 2$ mm with respect to only the depth. It is observed that the SAR at 61.22 GHz decreases at a higher rate along the depth of human skin compared to the SAR at 42.25 GHz. At depth of less than 0.3 mm, the human skin experiences more absorption at 61.22 GHz. Beyond 0.3 mm,

Figure 4.8: SAR of human skin at 42.25 GHz and 61.22 GHz with respect to depth.

the absorption at 42.25 GHz is more. Furthermore, beyond 1.5 mm which is the fat layer, the human skin has negligible absorption at both frequencies. This is due to the fact that most of the electromagnetic energy has already been absorbed in the epidermis and dermis layers of the human skin, which results in weak penetration of power into the fat layer.

For comparison, we have also computed the SAR using the efficient fundamental form of ADI-FDTD with averaging and forward-forward schemes. As reference, the same numerical example is performed using the Yee's explicit FDTD method of time-averaging scheme [2]. The normalized SAR error is defined as

$$SAR_{error} = \frac{SAR_{FADI} - SAR_{explicit}}{\max(SAR_{explicit})} \quad (4.8.8)$$

where SAR_{FADI} is the SAR computed using various efficient fundamental form of ADI-FDTD schemes and $SAR_{explicit}$ is the SAR computed using the Yee's explicit FDTD method. Figs. 4.9, 4.10 and 4.11 show the normalized SAR error of ETD, averaging and forward-forward schemes at 42.25 GHz and z cut plane of 2 mm. It is seen that the forward-forward scheme incurs the highest error due to the fact

Figure 4.9: Normalized SAR error with respect to depth and width at 42.25 GHz for ETD scheme.

that the scheme is only first-order in temporal accuracy. The ETD and averaging schemes are both second-order in temporal accuracy and thus, exhibits lower error.

4.9 FADI-FDTD Formulation for Various Dispersive Media Models

In this section, various dispersive media models are incorporated into the FADI-FDTD. The generalized formulation for conventional ADI-FDTD is first shown for doubly dispersive media, and will be extended into our efficient FADI-FDTD method. Such generalized formulation is then applied to Debye, Lorentz, Drude and complex conjugate pole-residue pair models. For convenience, all subscript indices in this chapter shall be dropped.

4.9.1 Generalized Formulation

For completeness, we include the formulation of both electric and magnetic dispersive media. The generalized formulation for dispersive media is first performed to the conventional ADI-FDTD method before being extended into FADI-FDTD

Figure 4.10: Normalized SAR error with respect to depth and width at 42.25 GHz for averaging scheme.

method. To that end, the generalized frequency domain electric and magnetic current densities of the p -th pole dispersive media, $\tilde{\mathbf{J}}_p^g(\omega)$ and $\tilde{\mathbf{M}}_p^g(\omega)$ are related to frequency domain electric and magnetic fields $\tilde{\mathbf{E}}(\omega)$ and $\tilde{\mathbf{H}}(\omega)$ by

$$\begin{aligned}\tilde{\mathbf{J}}_p^g(\omega) &= j\omega\epsilon_0\chi_{e,p}(\omega)\tilde{\mathbf{E}}(\omega) \\ &= \zeta_{e,p}^g(\omega)\tilde{\mathbf{E}}(\omega)\end{aligned}\tag{4.9.1a}$$

$$\begin{aligned}\tilde{\mathbf{M}}_p^g(\omega) &= j\omega\mu_0\chi_{h,p}(\omega)\tilde{\mathbf{H}}(\omega) \\ &= \zeta_{h,p}^g(\omega)\tilde{\mathbf{H}}(\omega)\end{aligned}\tag{4.9.1b}$$

where $\chi_{e,p}(\omega)$ and $\chi_{h,p}(\omega)$ are frequency domain electric and magnetic susceptibility function of p -th pole dispersive media respectively. $\zeta_{e,p}^g(\omega)$ and $\zeta_{h,p}^g(\omega)$ are the generalized electric and magnetic frequency domain transfer functions that relates $\tilde{\mathbf{J}}_p^g(\omega)$ and $\tilde{\mathbf{M}}_p^g(\omega)$ to $\tilde{\mathbf{E}}(\omega)$ and $\tilde{\mathbf{H}}(\omega)$ respectively.

These frequency domain transfer functions can be decomposed into two parts to yield:

$$\zeta_{e,p}^g(\omega)\tilde{\mathbf{E}}(\omega) = \left(\zeta_{e,p}(\omega) + \zeta'_{e,p}(\omega)\right)\tilde{\mathbf{E}}(\omega)$$

Figure 4.11: Normalized SAR error with respect to depth and width at 42.25 GHz for forward-forward scheme.

$$= \tilde{\mathbf{J}}_p(\omega) + \tilde{\mathbf{J}}'_p(\omega) \quad (4.9.2a)$$

$$\begin{aligned} \zeta_{h,p}^g(\omega) \tilde{\mathbf{H}}(\omega) &= (\zeta_{h,p}(\omega) + \zeta'_{h,p}(\omega)) \tilde{\mathbf{H}}(\omega) \\ &= \tilde{\mathbf{M}}_p(\omega) + \tilde{\mathbf{M}}'_p(\omega) \end{aligned} \quad (4.9.2b)$$

where

$$\tilde{\mathbf{J}}_p(\omega) = \zeta_{e,p}(\omega) \tilde{\mathbf{E}}(\omega) \quad (4.9.3a)$$

$$\tilde{\mathbf{J}}'_p(\omega) = \zeta'_{e,p}(\omega) \tilde{\mathbf{E}}(\omega) \quad (4.9.3b)$$

$$\tilde{\mathbf{M}}_p(\omega) = \zeta_{h,p}(\omega) \tilde{\mathbf{H}}(\omega) \quad (4.9.3c)$$

$$\tilde{\mathbf{M}}'_p(\omega) = \zeta'_{h,p}(\omega) \tilde{\mathbf{H}}(\omega) \quad (4.9.3d)$$

Note that in doing so, the generalized frequency domain electric current densities of the p -th pole dispersive media, $\tilde{\mathbf{J}}_p^g(\omega)$ is decomposed into $\tilde{\mathbf{J}}_p(\omega)$ and $\tilde{\mathbf{J}}'_p(\omega)$ while its magnetic counterpart is decomposed into $\tilde{\mathbf{M}}_p(\omega)$ and $\tilde{\mathbf{M}}'_p(\omega)$. The condition for the above decomposition will be shown later.

Taking the decomposition into consideration, we write down the Maxwell's curl

equations as

$$\begin{aligned}\nabla \times \mathbf{H}(t) &= \epsilon_0 \epsilon_\infty \frac{\partial}{\partial t} \mathbf{E}(t) + \sigma \mathbf{E}(t) + \sum_p \mathcal{F}^{-1} \left\{ \left(\zeta_{e,p}(\omega) + \zeta'_{e,p}(\omega) \right) \mathbf{E}(\omega) \right\} \\ &= \epsilon_0 \epsilon_\infty \frac{\partial}{\partial t} \mathbf{E}(t) + \sigma \mathbf{E}(t) + \sum_p \left(\mathbf{J}_p(t) + \mathbf{J}'_p(t) \right)\end{aligned}\quad (4.9.4a)$$

$$\begin{aligned}-\nabla \times \mathbf{E}(t) &= \mu_0 \mu_\infty \frac{\partial}{\partial t} \mathbf{H}(t) + \sigma^* \mathbf{H}(t) + \sum_p \mathcal{F}^{-1} \left\{ \left(\zeta_{h,p}(\omega) + \zeta'_{h,p}(\omega) \right) \mathbf{H}(\omega) \right\} \\ &= \mu_0 \mu_\infty \frac{\partial}{\partial t} \mathbf{H}(t) + \sigma^* \mathbf{H}(t) + \sum_p \left(\mathbf{M}_p(t) + \mathbf{M}'_p(t) \right)\end{aligned}\quad (4.9.4b)$$

where ϵ_∞ and μ_∞ are permittivity and permeability at infinite frequency respectively.

We now state the condition for the decomposition in (4.9.2). To guarantee real-valued time signal in (4.9.4), the following condition must hold:

$$\mathbf{J}_p(t) + \mathbf{J}'_p(t) = 2 \operatorname{Re} \{ \mathbf{J}_p(t) \} \quad (4.9.5a)$$

$$\mathbf{M}_p(t) + \mathbf{M}'_p(t) = 2 \operatorname{Re} \{ \mathbf{M}_p(t) \} \quad (4.9.5b)$$

For complex-valued $\mathbf{J}_p(t)$, we note that $\mathbf{J}'_p(t) = \mathbf{J}_p^*(t)$ where “*” denotes its complex conjugate. On the other hand, for real-valued $\mathbf{J}_p(t)$, $\mathbf{J}'_p(t) = \mathbf{J}_p(t)$. As will be shown later, the condition in (4.9.5) is true and applicable for complex conjugate pole-residue pair, Debye, Lorentz and Drude dispersive models.

Using the condition in (4.9.5), the Maxwell's curl equations can now be rewritten as

$$\nabla \times \mathbf{H}(t) = \epsilon_0 \epsilon_\infty \frac{\partial}{\partial t} \mathbf{E}(t) + \sigma \mathbf{E}(t) + \sum_p 2 \operatorname{Re} \{ \mathbf{J}_p(t) \} \quad (4.9.6a)$$

$$-\nabla \times \mathbf{E}(t) = \mu_0 \mu_\infty \frac{\partial}{\partial t} \mathbf{H}(t) + \sigma^* \mathbf{H}(t) + \sum_p 2 \operatorname{Re} \{ \mathbf{M}_p(t) \}. \quad (4.9.6b)$$

Since (4.9.5) holds true, we need only consider (4.9.3a) and (4.9.3c). Converting (4.9.3a) and (4.9.3c) into time domain, we let the generalized discretization formu-

lation in two substeps as

$$\mathbf{J}_p^{n+\frac{1}{2}} = k_{1p}\mathbf{J}_p^n + k_{2p}\mathbf{E}^{n+\frac{1}{2}} + k_{3p}\mathbf{E}^n \quad (4.9.7a)$$

$$\mathbf{M}_p^{n+\frac{1}{2}} = l_{1p}\mathbf{M}_p^n + l_{2p}\mathbf{H}^{n+\frac{1}{2}} + l_{3p}\mathbf{H}^n \quad (4.9.7b)$$

and

$$\mathbf{J}_p^{n+1} = k_{1p}\mathbf{J}_p^{n+\frac{1}{2}} + k_{2p}\mathbf{E}^{n+1} + k_{3p}\mathbf{E}^{n+\frac{1}{2}} \quad (4.9.8a)$$

$$\mathbf{M}_p^{n+1} = l_{1p}\mathbf{M}_p^{n+\frac{1}{2}} + l_{2p}\mathbf{H}^{n+1} + l_{3p}\mathbf{H}^{n+\frac{1}{2}}. \quad (4.9.8b)$$

Note that the discretization in two substeps is required in ADI-FDTD method.

We now discretize (4.9.6) into two substeps using ADI-FDTD method and combine it with semi-implicit approximation of

$$\frac{1}{2} \left(\mathbf{J}_p^n + \mathbf{J}_p^{n+\frac{1}{2}} \right) = \frac{1}{2} \left[(1 + k_{1p}) \mathbf{J}_p^n + k_{2p}\mathbf{E}^{n+\frac{1}{2}} + k_{3p}\mathbf{E}^n \right] \quad (4.9.9)$$

and

$$\frac{1}{2} \left(\mathbf{J}_p^{n+\frac{1}{2}} + \mathbf{J}_p^{n+1} \right) = \frac{1}{2} \left[(1 + k_{1p}) \mathbf{J}_p^{n+\frac{1}{2}} + k_{2p}\mathbf{E}^{n+1} + k_{3p}\mathbf{E}^{n+\frac{1}{2}} \right]. \quad (4.9.10)$$

Upon some manipulations, the generalized update equations of conventional ADI-FDTD method for dispersive media read:

For the first substep n to $n + \frac{1}{2}$:

$$E_x^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} H_z^{n+\frac{1}{2}} = c_1 E_x^n - c_2 \frac{\partial}{\partial z} H_y^n - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{xp}^n \right\} \quad (4.9.11a)$$

$$E_y^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial z} H_x^{n+\frac{1}{2}} = c_1 E_y^n - c_2 \frac{\partial}{\partial x} H_z^n - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{yp}^n \right\} \quad (4.9.11b)$$

$$E_z^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial x} H_y^{n+\frac{1}{2}} = c_1 E_z^n - c_2 \frac{\partial}{\partial y} H_x^n - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{zp}^n \right\} \quad (4.9.11c)$$

$$H_x^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial z} E_y^{n+\frac{1}{2}} = d_1 H_x^n - d_2 \frac{\partial}{\partial y} E_z^n - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{xp}^n \right\} \quad (4.9.11d)$$

$$H_y^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial x} E_z^{n+\frac{1}{2}} = d_1 H_y^n - d_2 \frac{\partial}{\partial z} E_x^n - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{yp}^n \right\} \quad (4.9.11e)$$

$$H_z^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}} = d_1 H_z^n - d_2 \frac{\partial}{\partial x} E_y^n - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{zp}^n \right\} \quad (4.9.11f)$$

$$J_{\xi p}^{n+\frac{1}{2}} = k_{1p} J_{\xi p}^n + k_{2p} E_{\xi}^{n+\frac{1}{2}} + k_{3p} E_{\xi}^n \quad \forall p, \quad \xi = x, y, z \quad (4.9.11g)$$

$$M_{\xi p}^{n+\frac{1}{2}} = l_{1p} M_{\xi p}^n + l_{2p} M_{\xi}^{n+\frac{1}{2}} + l_{3p} M_{\xi}^n \quad \forall p, \quad \xi = x, y, z \quad (4.9.11h)$$

For the second substep $n + \frac{1}{2}$ to $n + 1$:

$$E_x^{n+1} + c_2 \frac{\partial}{\partial z} H_y^{n+1} = c_1 E_x^{n+\frac{1}{2}} + c_2 \frac{\partial}{\partial y} H_z^{n+\frac{1}{2}} - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{xp}^{n+\frac{1}{2}} \right\} \quad (4.9.12a)$$

$$E_y^{n+1} + c_2 \frac{\partial}{\partial x} H_z^{n+1} = c_1 E_y^{n+\frac{1}{2}} + c_2 \frac{\partial}{\partial z} H_x^{n+\frac{1}{2}} - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{yp}^{n+\frac{1}{2}} \right\} \quad (4.9.12b)$$

$$E_z^{n+1} + c_2 \frac{\partial}{\partial y} H_x^{n+1} = c_1 E_z^{n+\frac{1}{2}} + c_2 \frac{\partial}{\partial x} H_y^{n+\frac{1}{2}} - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{zp}^{n+\frac{1}{2}} \right\} \quad (4.9.12c)$$

$$H_x^{n+1} + d_2 \frac{\partial}{\partial y} E_z^{n+1} = d_1 H_x^{n+\frac{1}{2}} + d_2 \frac{\partial}{\partial z} E_y^{n+\frac{1}{2}} - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{xp}^{n+\frac{1}{2}} \right\} \quad (4.9.12d)$$

$$H_y^{n+1} + d_2 \frac{\partial}{\partial z} E_x^{n+1} = d_1 H_y^{n+\frac{1}{2}} + d_2 \frac{\partial}{\partial x} E_z^{n+\frac{1}{2}} - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{yp}^{n+\frac{1}{2}} \right\} \quad (4.9.12e)$$

$$H_z^{n+1} + d_2 \frac{\partial}{\partial x} E_y^{n+1} = d_1 H_z^{n+\frac{1}{2}} + d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}} - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{zp}^{n+\frac{1}{2}} \right\} \quad (4.9.12f)$$

$$J_{\xi p}^{n+1} = k_{1p} J_{\xi p}^{n+\frac{1}{2}} + k_{2p} E_{\xi}^{n+1} + k_{3p} E_{\xi}^{n+\frac{1}{2}} \quad \forall p, \quad \xi = x, y, z \quad (4.9.12g)$$

$$M_{\xi p}^{n+1} = l_{1p} M_{\xi p}^{n+\frac{1}{2}} + l_{2p} H_{\xi}^{n+1} + l_{3p} H_{\xi}^{n+\frac{1}{2}} \quad \forall p, \quad \xi = x, y, z \quad (4.9.12h)$$

where

$$c_1 = \frac{1 - \frac{\sigma \Delta t}{4\epsilon_0 \epsilon_\infty} - \frac{\Delta t}{4\epsilon_0 \epsilon_\infty} \sum_p 2 \text{Re}(k_{3p})}{1 + \frac{\sigma \Delta t}{4\epsilon_0 \epsilon_\infty} + \frac{\Delta t}{4\epsilon_0 \epsilon_\infty} \sum_p 2 \text{Re}(k_{2p})}, \quad c_2 = \frac{\frac{\Delta t}{2\epsilon_0 \epsilon_\infty}}{1 + \frac{\sigma \Delta t}{4\epsilon_0 \epsilon_\infty} + \frac{\Delta t}{4\epsilon_0 \epsilon_\infty} \sum_p 2 \text{Re}(k_{2p})}, \quad (4.9.13a)$$

$$d_1 = \frac{1 - \frac{\sigma^* \Delta t}{4\mu_0 \mu_\infty} - \frac{\Delta t}{4\mu_0 \mu_\infty} \sum_p 2 \text{Re}(l_{3p})}{1 + \frac{\sigma^* \Delta t}{4\mu_0 \mu_\infty} + \frac{\Delta t}{4\mu_0 \mu_\infty} \sum_p 2 \text{Re}(l_{2p})}, \quad d_2 = \frac{\frac{\Delta t}{2\mu_0 \mu_\infty}}{1 + \frac{\sigma^* \Delta t}{4\mu_0 \mu_\infty} + \frac{\Delta t}{4\mu_0 \mu_\infty} \sum_p 2 \text{Re}(l_{2p})}. \quad (4.9.13b)$$

To solve for E_x in the first substep, we need to substitute (4.9.11f) into (4.9.11a) to obtain the implicit electric field update equation as

$$E_x^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} (d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}}) = c_1 E_x^n - c_2 \frac{\partial}{\partial z} H_y^n - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{xp}^n \right\} + c_2 \frac{\partial}{\partial y} (d_1 H_z^n)$$

$$-c_2 \frac{\partial}{\partial y} (d_2 \frac{\partial}{\partial x} E_y^n) - c_2 \frac{\partial}{\partial y} (d_2 \sum_p \text{Re} \{ (1 + l_{1p}) M_{xp}^n \}). \quad (4.9.14)$$

For E_y , (4.9.11d) is substituted into (4.9.11b) and for E_z , (4.9.11e) is substituted into (4.9.11c). After the E fields are solved, H , J and M fields can be obtained explicitly via (4.9.11d)-(4.9.11h). The procedures are then repeated for the second substep. When the spatial differential operators are approximated using the second-order central differencing operated on a standard Yee's cell [1], the electric field components can be obtained by solving a set of tridiagonal matrices.

The generalized update equations of conventional ADI-FDTD for dispersive media can be formulated into compact matrix form (in two substeps) as

$$(\mathbf{I}_{18} - \mathbf{D}_2 \mathbf{A} + \mathbf{F}_l) \mathbf{u}^{n+\frac{1}{2}} = (\mathbf{D}_1 + \mathbf{D}_2 \mathbf{B} + \mathbf{F}_r) \mathbf{u}^n + \mathbf{D}_2 \mathbf{s}^{n+\frac{1}{2}} \quad (4.9.15a)$$

$$(\mathbf{I}_{18} - \mathbf{D}_2 \mathbf{B} + \mathbf{F}_l) \mathbf{u}^{n+1} = (\mathbf{D}_1 + \mathbf{D}_2 \mathbf{A} + \mathbf{F}_r) \mathbf{u}^{n+\frac{1}{2}} + \mathbf{D}_2 \mathbf{s}^{n+\frac{1}{2}} \quad (4.9.15b)$$

where

$$\mathbf{u} = [E_x, E_y, E_z, H_x, H_y, H_z, J_x^r, J_y^r, J_z^r, J_x^i, J_y^i, J_z^i, M_x^r, M_y^r, M_z^r, M_x^i, M_y^i, M_z^i]^T \quad (4.9.16)$$

$$\mathbf{s} = [-s_{ex}, -s_{ey}, -s_{ez}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]^T \quad (4.9.17)$$

$$\mathbf{A} = \begin{bmatrix} \mathbf{O}_3 & \mathbf{K}_1 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{K}_2 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} \mathbf{O}_3 & -\mathbf{K}_2 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ -\mathbf{K}_1 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \end{bmatrix} \quad (4.9.18)$$

$$\mathbf{K}_1 = \begin{bmatrix} 0 & 0 & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & 0 \\ 0 & \frac{\partial}{\partial x} & 0 \end{bmatrix}, \quad \mathbf{K}_2 = \begin{bmatrix} 0 & \frac{\partial}{\partial z} & 0 \\ 0 & 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} & 0 & 0 \end{bmatrix} \quad (4.9.19)$$

$$\mathbf{D}_1 = \text{diag}(c_1, c_1, c_1, d_1, d_1, d_1, k_1^r, k_1^r, k_1^r, k_1^r, k_1^r, k_1^r, l_1^r, l_1^r, l_1^r, l_1^r, l_1^r, l_1^r) \quad (4.9.20)$$

$$\mathbf{D}_2 = \text{diag}(c_2, c_2, c_2, d_2, d_2, d_2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \quad (4.9.21)$$

$$\mathbf{F}_l = \begin{bmatrix} \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ -k_2^r \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ -k_2^i \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & -l_2^r \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & -l_2^i \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \end{bmatrix} \quad (4.9.22)$$

$$\mathbf{F}_r = \begin{bmatrix} \mathbf{O}_3 & \mathbf{O}_3 & -c_2(1 + k_1^r) \mathbf{I}_3 & c_2 k_1^i \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & -d_2(1 + l_1^r) \mathbf{I}_3 & d_2 l_1^i \mathbf{I}_3 \\ k_3^r \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & -k_1^i \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ k_3^i \mathbf{I}_3 & \mathbf{O}_3 & k_1^r \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & l_3^r \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & -l_1^i \mathbf{I}_3 \\ \mathbf{O}_3 & l_3^i \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & l_1^r \mathbf{I}_3 & \mathbf{O}_3 \end{bmatrix}. \quad (4.9.23)$$

Note that any variables ρ^r represents $\text{Re}(\rho)$ and on the other hand ρ^i represents $\text{Im}(\rho)$. For simplicity, we assume only single pole of dispersive media for now. $\mathbf{I}_r$ and $\mathbf{O}_r$ represent identity and null matrices with dimension $r \times r$. We have also included electric current sources s_{ex} , s_{ey} and s_{ez} in the formulation.

A quick glance at (4.9.15) shows that its RHS still involves matrix operators $\mathbf{A}$ and $\mathbf{B}$ which incur considerable arithmetic operations and memory indexing, especially

when one is solving the implicit update equations. Efforts have been made to further reduce such overheads by means of a more efficient ADI-FDTD method in lossless media proposed in [120, 121]. Such efficient ADI algorithm is included within a family of fundamental implicit schemes, which feature similar fundamental updating structures that are in simplest forms with most efficient matrix-operator-free RHS. We now present the formulation of FADI-FDTD method for dispersive media.

Introducing an auxiliary variable $\hat{\mathbf{v}}$, (4.9.15) is rewritten as

$$\hat{\mathbf{v}}^n = (\mathbf{D}_1 + \mathbf{D}_2\mathbf{B} + \mathbf{F}_r) \mathbf{u}^n \quad (4.9.24a)$$

$$(\mathbf{I}_{18} - \mathbf{D}_2\mathbf{A} + \mathbf{F}_l) \mathbf{u}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^n + \mathbf{D}_2\mathbf{s}^{n+\frac{1}{2}} \quad (4.9.24b)$$

$$\hat{\mathbf{v}}^{n+\frac{1}{2}} = (\mathbf{D}_1 + \mathbf{D}_2\mathbf{A} + \mathbf{F}_r) \mathbf{u}^{n+\frac{1}{2}} + \mathbf{D}_2\mathbf{s}^{n+\frac{1}{2}} \quad (4.9.24c)$$

$$(\mathbf{I}_{18} - \mathbf{D}_2\mathbf{B} + \mathbf{F}_l) \mathbf{u}^{n+1} = \hat{\mathbf{v}}^{n+\frac{1}{2}} \quad (4.9.24d)$$

Next, (4.9.24d) is expressed at one time step backward as

$$\hat{\mathbf{v}}^{n-\frac{1}{2}} = (\mathbf{I}_{18} - \mathbf{D}_2\mathbf{B} + \mathbf{F}_l) \mathbf{u}^n \quad (4.9.25)$$

and (4.9.24a) can be subsequently reduced into

$$\begin{aligned} \hat{\mathbf{v}}^n &= (\mathbf{D}_1 + \mathbf{D}_2\mathbf{B} + \mathbf{F}_r) \mathbf{u}^n \\ &= [(\mathbf{I}_{18} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^n - (\mathbf{I}_{18} - \mathbf{D}_2\mathbf{B} + \mathbf{F}_l) \mathbf{u}^n \\ &= [(\mathbf{I}_{18} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^n - \hat{\mathbf{v}}^{n-\frac{1}{2}} \end{aligned} \quad (4.9.26)$$

Similarly, by rewriting (4.9.24b) as

$$\hat{\mathbf{v}}^n = (\mathbf{I}_{18} - \mathbf{D}_2\mathbf{A} + \mathbf{F}_l) \mathbf{u}^{n+\frac{1}{2}} - \mathbf{D}_2\mathbf{s}^{n+\frac{1}{2}}, \quad (4.9.27)$$

(4.9.24c) is reducible to

$$\hat{\mathbf{v}}^{n+\frac{1}{2}} = (\mathbf{D}_1 + \mathbf{D}_2\mathbf{A} + \mathbf{F}_r) \mathbf{u}^{n+\frac{1}{2}} + \mathbf{D}_2\mathbf{s}^{n+\frac{1}{2}}$$

$$\begin{aligned}
&= [(\mathbf{I}_{18} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^{n+\frac{1}{2}} - [(\mathbf{I}_{18} - \mathbf{D}_2 \mathbf{A} + \mathbf{F}_l) \mathbf{u}^{n+\frac{1}{2}} - \mathbf{D}_2 \mathbf{s}^{n+\frac{1}{2}}] \\
&= [(\mathbf{I}_{18} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^{n+\frac{1}{2}} - \hat{\mathbf{v}}^n
\end{aligned} \tag{4.9.28}$$

Finally, the FADI-FDTD update procedures read:

$$\hat{\mathbf{v}}^n = [(\mathbf{I}_{12} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^n - \hat{\mathbf{v}}^{n-\frac{1}{2}} \tag{4.9.29a}$$

$$(\mathbf{I}_{12} - \mathbf{D}_2 \mathbf{A} + \mathbf{F}_l) \mathbf{u}^{n+\frac{1}{2}} = \hat{\mathbf{v}}^n + \mathbf{D}_2 \mathbf{s}^{n+\frac{1}{2}} \tag{4.9.29b}$$

$$\hat{\mathbf{v}}^{n+\frac{1}{2}} = [(\mathbf{I}_{12} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^{n+\frac{1}{2}} - \hat{\mathbf{v}}^n \tag{4.9.29c}$$

$$(\mathbf{I}_{12} - \mathbf{D}_2 \mathbf{B} + \mathbf{F}_l) \mathbf{u}^{n+1} = \hat{\mathbf{v}}^{n+\frac{1}{2}} \tag{4.9.29d}$$

where (4.9.29a) and (4.9.29b) form the first substep while (4.9.29c) and (4.9.29d) form the second. It is worth noting that the FADI-FDTD has matrix-operator-free RHS, i.e., there is no matrix operator $\mathbf{A}$ and $\mathbf{B}$ on the RHS of (4.9.29). The source excitation is also only needed at the first substep [65] which further simplifies the implementation compared to the conventional ADI-FDTD method.

We now provide the full update equations of FADI-FDTD by expanding (4.9.29).

Letting

$$\hat{\mathbf{v}} = [\hat{e}_x, \hat{e}_y, \hat{e}_z, \hat{h}_x, \hat{h}_y, \hat{h}_z, \hat{j}_x^r, \hat{j}_y^r, \hat{j}_z^r, \hat{j}_x^i, \hat{j}_y^i, \hat{j}_z^i, \hat{m}_x^r, \hat{m}_y^r, \hat{m}_z^r, \hat{m}_x^i, \hat{m}_y^i, \hat{m}_z^i]^T, \tag{4.9.30}$$

and extending for arbitrary p dispersive pole, the full generalized update equations of FADI-FDTD method for dispersive media read:

For the first substep from n to $n + \frac{1}{2}$:

$$\hat{e}_\xi^n = (1 + c_1) E_\xi^n - \hat{e}_x^{n-\frac{1}{2}} - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{\xi p}^n \right\}, \quad \xi = x, y, z \tag{4.9.31a}$$

$$\hat{h}_\xi^n = (1 + d_1) H_\xi^n - \hat{h}_x^{n-\frac{1}{2}} - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{\xi p}^n \right\}, \quad \xi = x, y, z \tag{4.9.31b}$$

$$\hat{j}_{\xi p}^n = (1 + k_{1p}) J_{\xi p}^n - \hat{j}_{\xi p}^{n-\frac{1}{2}} + (k_{3p} - k_{2p}) E_\xi^n, \quad \forall p, \quad \xi = x, y, z \tag{4.9.31c}$$

$$\hat{m}_{\xi p}^n = (1 + l_{1p}) M_{\xi p}^n - \hat{m}_{\xi p}^{n-\frac{1}{2}} + (l_{3p} - l_{2p}) H_\xi^n, \quad \forall p, \quad \xi = x, y, z \tag{4.9.31d}$$

$$E_x^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} H_z^{n+\frac{1}{2}} = \hat{e}_x^n - c_2 s_{ex} \quad (4.9.31e)$$

$$E_y^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial z} H_x^{n+\frac{1}{2}} = \hat{e}_y^n - c_2 s_{ey} \quad (4.9.31f)$$

$$E_z^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial x} H_y^{n+\frac{1}{2}} = \hat{e}_z^n - c_2 s_{ez} \quad (4.9.31g)$$

$$H_x^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial z} E_y^{n+\frac{1}{2}} = \hat{h}_x^n \quad (4.9.31h)$$

$$H_y^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial x} E_z^{n+\frac{1}{2}} = \hat{h}_y^n \quad (4.9.31i)$$

$$H_z^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}} = \hat{h}_z^n \quad (4.9.31j)$$

$$J_{\xi p}^{n+\frac{1}{2}} = k_{2p} E_{\xi}^{n+\frac{1}{2}} + \hat{j}_{\xi p}^n, \quad \forall p, \quad \xi = x, y, z \quad (4.9.31k)$$

$$M_{\xi p}^{n+\frac{1}{2}} = l_{2p} H_{\xi}^{n+\frac{1}{2}} + \hat{m}_{\xi p}^n, \quad \forall p, \quad \xi = x, y, z. \quad (4.9.31l)$$

For second substep from $n + \frac{1}{2}$ to $n + 1$:

$$\hat{e}_{\xi}^{n+\frac{1}{2}} = (1 + c_1) E_{\xi}^{n+\frac{1}{2}} - \hat{e}_{\xi}^n - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p}) J_{\xi p}^{n+\frac{1}{2}} \right\}, \quad \xi = x, y, z \quad (4.9.32a)$$

$$\hat{h}_{\xi}^{n+\frac{1}{2}} = (1 + d_1) H_{\xi}^{n+\frac{1}{2}} - \hat{h}_{\xi}^n - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p}) M_{\xi p}^n \right\}, \quad \xi = x, y, z \quad (4.9.32b)$$

$$\hat{j}_{\xi p}^{n+\frac{1}{2}} = (1 + k_{1p}) J_{\xi p}^{n+\frac{1}{2}} - \hat{j}_{\xi p}^n + (k_{3p} - k_{2p}) E_{\xi}^{n+\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z \quad (4.9.32c)$$

$$\hat{m}_{\xi p}^{n+\frac{1}{2}} = (1 + l_{1p}) M_{\xi p}^{n+\frac{1}{2}} - \hat{m}_{\xi p}^n + (l_{3p} - l_{2p}) H_{\xi}^{n+\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z \quad (4.9.32d)$$

$$E_x^{n+1} + c_2 \frac{\partial}{\partial z} H_y^{n+1} = \hat{e}_x^{n+\frac{1}{2}} \quad (4.9.32e)$$

$$E_y^{n+1} + c_2 \frac{\partial}{\partial x} H_z^{n+1} = \hat{e}_y^{n+\frac{1}{2}} \quad (4.9.32f)$$

$$E_z^{n+1} + c_2 \frac{\partial}{\partial y} H_x^{n+1} = \hat{e}_z^{n+\frac{1}{2}} \quad (4.9.32g)$$

$$H_x^{n+1} + d_2 \frac{\partial}{\partial y} E_z^{n+1} = \hat{h}_x^{n+\frac{1}{2}} \quad (4.9.32h)$$

$$H_y^{n+1} + d_2 \frac{\partial}{\partial z} E_x^{n+1} = \hat{h}_y^{n+\frac{1}{2}} \quad (4.9.32i)$$

$$H_z^{n+1} + d_2 \frac{\partial}{\partial x} E_y^{n+1} = \hat{h}_z^{n+\frac{1}{2}} \quad (4.9.32j)$$

$$J_{\xi p}^{n+1} = k_{2p} E_{\xi}^{n+1} + \hat{j}_{\xi p}^{n+\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z \quad (4.9.32k)$$

$$M_{\xi p}^{n+1} = l_{2p} H_{\xi}^{n+1} + \hat{m}_{\xi p}^{n+\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z. \quad (4.9.32l)$$

Since J and M fields are not required in output, (4.9.31k) and (4.9.31l) can be further substituted into (4.9.32a), (4.9.32b), (4.9.32c) and (4.9.32d) for more efficiency and simplicity to yield

$$\begin{aligned} \hat{e}_\xi^{n+\frac{1}{2}} = & \left[1 + c_1 - c_2 \sum_p \operatorname{Re} \{ (1 + k_{1p}) k_{2p} \} \right] E_\xi^{n+\frac{1}{2}} - \hat{e}_\xi^n \\ & - c_2 \sum_p \operatorname{Re} \{ (1 + k_{1p}) \hat{j}_{\xi p}^n \} \end{aligned} \quad (4.9.33)$$

$$\begin{aligned} \hat{h}_\xi^{n+\frac{1}{2}} = & \left[1 + d_1 - d_2 \sum_p \operatorname{Re} \{ (1 + l_{1p}) l_{2p} \} \right] H_\xi^{n+\frac{1}{2}} - \hat{h}_\xi^n \\ & - c_2 \sum_p \operatorname{Re} \{ (1 + l_{1p}) \hat{m}_{\xi p}^n \} \end{aligned} \quad (4.9.34)$$

$$\hat{j}_{\xi p}^{n+\frac{1}{2}} = (k_{1p} k_{2p} + k_{3p}) E_\xi^{n+\frac{1}{2}} + k_{1p} \hat{j}_{\xi p}^n, \quad \forall p, \quad \xi = x, y, z \quad (4.9.35)$$

$$\hat{m}_{\xi p}^{n+\frac{1}{2}} = (l_{1p} l_{2p} + l_{3p}) H_\xi^{n+\frac{1}{2}} + l_{1p} \hat{m}_{\xi p}^n, \quad \forall p, \quad \xi = x, y, z \quad (4.9.36)$$

Similarly, (4.9.32k) and (4.9.32l) at one time step earlier can be further substituted into (4.9.31a), (4.9.31b), (4.9.31c) and (4.9.31d) to yield

$$\begin{aligned} \hat{e}_\xi^n = & \left[1 + c_1 - c_2 \sum_p \operatorname{Re} \{ (1 + k_{1p}) k_{2p} \} \right] E_\xi^n - \hat{e}_\xi^{n-\frac{1}{2}} \\ & - c_2 \sum_p \operatorname{Re} \{ (1 + k_{1p}) \hat{j}_{\xi p}^{n-\frac{1}{2}} \} \end{aligned} \quad (4.9.37)$$

$$\begin{aligned} \hat{h}_\xi^n = & \left[1 + d_1 - d_2 \sum_p \operatorname{Re} \{ (1 + l_{1p}) l_{2p} \} \right] H_\xi^n - \hat{h}_\xi^{n-\frac{1}{2}} \\ & - c_2 \sum_p \operatorname{Re} \{ (1 + l_{1p}) \hat{m}_{\xi p}^{n-\frac{1}{2}} \} \end{aligned} \quad (4.9.38)$$

$$\hat{j}_{\xi p}^n = (k_{1p} k_{2p} + k_{3p}) E_\xi^n + k_{1p} \hat{j}_{\xi p}^{n-\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z \quad (4.9.39)$$

$$\hat{m}_{\xi p}^n = (l_{1p} l_{2p} + l_{3p}) H_\xi^n + l_{1p} \hat{m}_{\xi p}^{n-\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z \quad (4.9.40)$$

To solve for E_x in the first substep implicitly, (4.9.31j) is substituted into (4.9.31e) to yield

$$E_x^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} \left(d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}} \right) = \hat{e}_x^n - c_2 s_{ex} + c_2 \frac{\partial}{\partial y} \hat{h}_z^n. \quad (4.9.41)$$

For E_y , (4.9.31h) is substituted into (4.9.31f) and for E_z , (4.9.31i) is substituted into (4.9.31g). Other field components are solved explicitly. The procedures are then repeated for the second substep.

The advantages of the FADI-FDTD over the conventional ADI-FDTD can be summarized as follows:

- 1) Matrix-operator-free RHS in FADI-FDTD, c.f. (4.9.29). On the other hand, the RHS of conventional ADI-FDTD still involves matrix operators $\mathbf{A}$ and $\mathbf{B}$, c.f. (4.9.15).
- 2) Source excitation is only needed in first substep of FADI-FDTD, c.f. (4.9.29b), compared to both substeps of conventional ADI-FDTD, c.f. (4.9.15a) and (4.9.15b).
- 3) Implicit update equation of FADI-FDTD, c.f. (4.9.41) is much simpler compared to that of conventional ADI-FDTD, c.f. (4.9.14).
- 4) Implicit update equation of FADI-FDTD, c.f. (4.9.41) has much lesser spatial differential operators than that of conventional ADI-FDTD, c.f. (4.9.14). Thus, applying finite difference approximation to these spatial differential operators will incur less overheads in FADI-FDTD compared to conventional ADI-FDTD.
- 5) No dispersive terms J and M is required in implicit update equation of FADI-FDTD, c.f. (4.9.41). On the other hand, they are required in implicit update equation of conventional ADI-FDTD, c.f. (4.9.14).
- 6) The overall number of RHS terms in FADI-FDTD are lesser than that of conventional ADI-FDTD. This reduces the amount of arithmetic operations, memory indexing, and results in higher efficiency.

4.9.2 Complex Conjugate Pole-Residue Pair

For complex conjugate pole-residue pair model, the frequency domain electric and magnetic susceptibility functions of the p -th pole are given as

$$\chi_{e,p} = \frac{r_p}{j\omega - a_p} + \frac{r_p^*}{j\omega - a_p^*} \quad (4.9.42a)$$

$$\chi_{h,p} = \frac{q_p}{j\omega - b_p} + \frac{q_p^*}{j\omega - b_p^*} \quad (4.9.42b)$$

where a_p and b_p are the p -th electric and magnetic poles respectively, r_p and q_p are the p -th pole electric and magnetic residues respectively.

From (4.9.1), the generalized electric and magnetic frequency domain transfer functions read:

$$\zeta_{e,p}^g(\omega) = j\omega\epsilon_0 \left(\frac{r_p}{j\omega - a_p} + \frac{r_p^*}{j\omega - a_p^*} \right) \quad (4.9.43a)$$

$$\zeta_{h,p}^g(\omega) = j\omega\mu_0 \left(\frac{q_p}{j\omega - b_p} + \frac{q_p^*}{j\omega - b_p^*} \right) \quad (4.9.43b)$$

In order to satisfy (4.9.5), $\zeta_{e,p}^g(\omega)$ and $\zeta_{h,p}^g(\omega)$ are decomposed into

$$\zeta_{e,p}(\omega) = \frac{j\omega\epsilon_0 r_p}{j\omega - a_p} \quad (4.9.44a)$$

$$\zeta'_{e,p}(\omega) = \frac{j\omega\epsilon_0 r_p^*}{j\omega - a_p^*} \quad (4.9.44b)$$

$$\zeta_{h,p}(\omega) = \frac{j\omega\mu_0 q_p}{j\omega - b_p} \quad (4.9.44c)$$

$$\zeta'_{h,p}(\omega) = \frac{j\omega\mu_0 q_p^*}{j\omega - b_p^*} \quad (4.9.44d)$$

and since (4.9.5) is true, we need only consider the relations in (4.9.3a) and (4.9.3c).

$\tilde{\mathbf{J}}_p(\omega)$ and $\tilde{\mathbf{M}}_p(\omega)$ are now related to $\tilde{\mathbf{E}}(\omega)$ and $\tilde{\mathbf{H}}(\omega)$ by

$$\tilde{\mathbf{J}}_p(\omega) = \frac{j\omega\epsilon_0 r_p}{j\omega - a_p} \tilde{\mathbf{E}}(\omega) \quad (4.9.45a)$$

$$\tilde{\mathbf{M}}_p(\omega) = \frac{j\omega\mu_0 q_p}{j\omega - b_p} \tilde{\mathbf{H}}(\omega) \quad (4.9.45b)$$

(4.9.45) can then converted into time domain as

$$\frac{\partial}{\partial t} \mathbf{J}_p(t) - a_p \mathbf{J}_p(t) = \epsilon_0 r_p \frac{\partial}{\partial t} \mathbf{E}(t) \quad (4.9.46a)$$

$$\frac{\partial}{\partial t} \mathbf{M}_p(t) - b_p \mathbf{M}_p(t) = \mu_0 q_p \frac{\partial}{\partial t} \mathbf{H}(t). \quad (4.9.46b)$$

Discretizing (4.9.46) using central difference approximation, the update coefficients in (4.9.7) and (4.9.8) is found to be

$$k_{1p} = \frac{1 + a_p \frac{\Delta t}{4}}{1 - a_p \frac{\Delta t}{4}}; \quad k_{2p} = \frac{r_p}{1 - a_p \frac{\Delta t}{4}}; \quad k_{3p} = -k_{2p}; \quad (4.9.47a)$$

$$l_{1p} = \frac{1 + b_p \frac{\Delta t}{4}}{1 - b_p \frac{\Delta t}{4}}; \quad l_{2p} = \frac{q_p}{1 - b_p \frac{\Delta t}{4}}; \quad l_{3p} = -l_{2p}; \quad (4.9.47b)$$

Once the update coefficients k_{1p} , k_{2p} , k_{3p} , l_{1p} , l_{2p} and l_{3p} are determined, the update equations of FADI-FDTD follows that of the generalized formulation detailed earlier.

4.9.3 Debye

For Debye model, the frequency domain electric and magnetic susceptibility functions of the p -th pole are given as

$$\chi_{e,p} = \frac{\Delta\epsilon_p}{1 + j\omega\tau_{e,p}} \quad (4.9.48a)$$

$$\chi_{h,p} = \frac{\Delta\mu_p}{1 + j\omega\tau_{h,p}} \quad (4.9.48b)$$

where $\Delta\epsilon_p$ and $\Delta\mu_p$ are change in relative permittivity and permeability respectively due to the p -th Debye pole, $\tau_{e,p}$ and $\tau_{h,p}$ are the p -th pole electric and magnetic relaxation times respectively.

From (4.9.1), the generalized electric and magnetic frequency domain transfer functions read:

$$\zeta_{e,p}^g(\omega) = j\omega\epsilon_0 \left(\frac{\Delta\epsilon_p}{1 + j\omega\tau_{e,p}} \right) \quad (4.9.49a)$$

$$\zeta_{h,p}^g(\omega) = j\omega\mu_0 \left(\frac{\Delta\mu_p}{1 + j\omega\tau_{h,p}} \right) \quad (4.9.49b)$$

In order to satisfy (4.9.5), $\zeta_{e,p}^g(\omega)$ and $\zeta_{h,p}^g(\omega)$ are decomposed into

$$\zeta_{e,p}(\omega) = \frac{j\omega\epsilon_0\Delta\epsilon_p/2}{1 + j\omega\tau_{e,p}} \quad (4.9.50a)$$

$$\zeta'_{e,p}(\omega) = \frac{j\omega\epsilon_0\Delta\epsilon_p/2}{1 + j\omega\tau_{e,p}} \quad (4.9.50b)$$

$$\zeta_{h,p}(\omega) = \frac{j\omega\mu_0\Delta\mu_p/2}{1 + j\omega\tau_{h,p}} \quad (4.9.50c)$$

$$\zeta'_{h,p}(\omega) = \frac{j\omega\mu_0\Delta\mu_p/2}{1 + j\omega\tau_{h,p}} \quad (4.9.50d)$$

and since (4.9.5) is true, we need only consider the relations in (4.9.3a) and (4.9.3c).

$\tilde{\mathbf{J}}_p(\omega)$ and $\tilde{\mathbf{M}}_p(\omega)$ are now related to $\tilde{\mathbf{E}}(\omega)$ and $\tilde{\mathbf{H}}(\omega)$ by

$$\tilde{\mathbf{J}}_p(\omega) = \frac{j\omega\epsilon_0\Delta\epsilon_p/2}{1 + j\omega\tau_{e,p}} \tilde{\mathbf{E}}(\omega) \quad (4.9.51a)$$

$$\tilde{\mathbf{M}}_p(\omega) = \frac{j\omega\mu_0\Delta\mu_p/2}{1 + j\omega\tau_{h,p}} \tilde{\mathbf{H}}(\omega) \quad (4.9.51b)$$

(4.9.45) can then converted into time domain as

$$\tau_{e,p} \frac{\partial}{\partial t} \mathbf{J}_p(t) + \mathbf{J}_p(t) = \frac{\epsilon_0\Delta\epsilon_p}{2} \frac{\partial}{\partial t} \mathbf{E}(t) \quad (4.9.52a)$$

$$\tau_{h,p} \frac{\partial}{\partial t} \mathbf{M}_p(t) + \mathbf{M}_p(t) = \frac{\mu_0\Delta\mu_p}{2} \frac{\partial}{\partial t} \mathbf{H}(t). \quad (4.9.52b)$$

Discretizing (4.9.46) using central difference approximation, the update coefficients in (4.9.7) and (4.9.8) is found to be

$$k_{1p} = \frac{1 - \frac{\Delta t}{4\tau_{e,p}}}{1 + \frac{\Delta t}{4\tau_{e,p}}}; \quad k_{2p} = \frac{\epsilon_0\Delta\epsilon_p/(2\tau_{e,p})}{1 + \frac{\Delta t}{4\tau_{e,p}}}; \quad k_{3p} = -k_{2p}; \quad (4.9.53a)$$

$$l_{1p} = \frac{1 - \frac{\Delta t}{4\tau_{h,p}}}{1 + \frac{\Delta t}{4\tau_{h,p}}}; \quad l_{2p} = \frac{\mu_0\Delta\mu_p/(2\tau_{h,p})}{1 + \frac{\Delta t}{4\tau_{h,p}}}; \quad l_{3p} = -l_{2p}; \quad (4.9.53b)$$

4.9.4 Lorentz

For Lorentz model, the frequency domain electric and magnetic susceptibility functions of the p -th pole are given as

$$\chi_{e,p} = \frac{\Delta\epsilon_p \omega_{e,p}^2}{\omega_{e,p}^2 + 2j\omega\delta_{e,p} - \omega^2} \quad (4.9.54a)$$

$$\chi_{h,p} = \frac{\Delta\mu_p \omega_{h,p}^2}{\omega_{h,p}^2 + 2j\omega\delta_{h,p} - \omega^2} \quad (4.9.54b)$$

where $\Delta\epsilon_p$ and $\Delta\mu_p$ are change in relative permittivity and permeability respectively due to the p -th Lorentz pole, $\omega_{e,p}$ and $\omega_{h,p}$ are the electric and magnetic resonant frequencies of the p -th pole respectively, $\delta_{e,p}$ and $\delta_{h,p}$ are the electric and magnetic damping coefficients of the p -th pole respectively.

The Lorentz model is in fact a complex conjugate pole-residue pair model which can be rewritten as

$$\frac{\Delta\epsilon_p \omega_{e,p}^2}{\omega_{e,p}^2 + 2j\omega\delta_{e,p} - \omega^2} = \frac{j\gamma_{e,p}/2}{j\omega + \alpha_{e,p} + j\beta_{e,p}} + \frac{-j\gamma_{e,p}/2}{j\omega + \alpha_{e,p} - j\beta_{e,p}} \quad (4.9.55a)$$

$$\frac{\Delta\mu_p \omega_{h,p}^2}{\omega_{h,p}^2 + 2j\omega\delta_{h,p} - \omega^2} = \frac{j\gamma_{h,p}/2}{j\omega + \alpha_{h,p} + j\beta_{h,p}} + \frac{-j\gamma_{h,p}/2}{j\omega + \alpha_{h,p} - j\beta_{h,p}} \quad (4.9.55b)$$

where

$$\alpha_{e,p} = \delta_{e,p}; \quad \beta_{e,p} = \sqrt{\omega_{e,p}}; \quad \gamma_{e,p} = \frac{\Delta\epsilon_p \omega_{e,p}^2}{\beta_{e,p}}; \quad (4.9.56a)$$

$$\alpha_{h,p} = \delta_{h,p}; \quad \beta_{h,p} = \sqrt{\omega_{h,p}}; \quad \gamma_{h,p} = \frac{\Delta\mu_p \omega_{h,p}^2}{\beta_{h,p}}. \quad (4.9.56b)$$

Comparing (4.9.55) to (4.9.42), we find that

$$a_p = -\alpha_{e,p} - j\beta_{e,p}; \quad r_p = j\gamma_{e,p}/2; \quad (4.9.57a)$$

$$b_p = -\alpha_{h,p} - j\beta_{h,p}; \quad q_p = j\gamma_{h,p}/2; \quad (4.9.57b)$$

The update coefficients k_{1p} , k_{2p} , k_{3p} , l_{1p} , l_{2p} and l_{3p} can then be determined from

(4.9.47) by replacing the poles and residues with the expressions in (4.9.57).

4.9.5 Drude

For Drude model, the frequency domain electric and magnetic susceptibility functions of the p -th pole are given as

$$\chi_{e,p} = \frac{-\omega_{e,p}^2}{\omega^2 - j\omega\nu_{e,p}} \quad (4.9.58a)$$

$$\chi_{h,p} = \frac{-\omega_{h,p}^2}{\omega^2 - j\omega\nu_{h,p}} \quad (4.9.58b)$$

where $\omega_{e,p}$ and $\omega_{h,p}$ are the p -th Drude pole electric and magnetic frequencies respectively. $\nu_{e,p}$ and $\nu_{h,p}$ are the inverse of the p -th pole electric and magnetic relaxation times respectively.

From (4.9.1), the generalized electric and magnetic frequency domain transfer functions read:

$$\begin{aligned} \zeta_{e,p}^g(\omega) &= j\omega\epsilon_0 \left(\frac{-\omega_{e,p}^2}{\omega^2 - j\omega\nu_{e,p}} \right) \\ &= \frac{\epsilon_0\omega_{e,p}^2}{j\omega + \nu_{e,p}} \end{aligned} \quad (4.9.59a)$$

$$\begin{aligned} \zeta_{h,p}^g(\omega) &= j\omega\mu_0 \left(\frac{-\omega_{h,p}^2}{\omega^2 - j\omega\nu_{h,p}} \right) \\ &= \frac{\epsilon_0\omega_{h,p}^2}{j\omega + \nu_{h,p}} \end{aligned} \quad (4.9.59b)$$

In order to satisfy (4.9.5), $\zeta_{e,p}^g(\omega)$ and $\zeta_{h,p}^g(\omega)$ are decomposed into

$$\zeta_{e,p}(\omega) = \frac{\epsilon_0\omega_{e,p}^2/2}{j\omega + \nu_{e,p}} \quad (4.9.60a)$$

$$\zeta'_{e,p}(\omega) = \frac{\epsilon_0\omega_{e,p}^2/2}{j\omega + \nu_{e,p}} \quad (4.9.60b)$$

$$\zeta_{h,p}(\omega) = \frac{\epsilon_0\omega_{h,p}^2/2}{j\omega + \nu_{h,p}} \quad (4.9.60c)$$

$$\zeta'_{h,p}(\omega) = \frac{\epsilon_0 \omega_{h,p}^2 / 2}{j\omega + \nu_{h,p}} \quad (4.9.60d)$$

and since (4.9.5) is true, we need only consider the relations in (4.9.3a) and (4.9.3c).

$\tilde{\mathbf{J}}_p(\omega)$ and $\tilde{\mathbf{M}}_p(\omega)$ are now related to $\tilde{\mathbf{E}}(\omega)$ and $\tilde{\mathbf{H}}(\omega)$ by

$$\tilde{\mathbf{J}}_p(\omega) = \frac{\epsilon_0 \omega_{e,p}^2 / 2}{j\omega + \nu_{e,p}} \tilde{\mathbf{E}}(\omega) \quad (4.9.61a)$$

$$\tilde{\mathbf{M}}_p(\omega) = \frac{\epsilon_0 \omega_{h,p}^2 / 2}{j\omega + \nu_{h,p}} \tilde{\mathbf{H}}(\omega) \quad (4.9.61b)$$

(4.9.45) can then be converted into time domain as

$$\frac{\partial}{\partial t} \mathbf{J}_p(t) + \nu_{e,p} \mathbf{J}_p(t) = \frac{\epsilon_0 \omega_{e,p}^2}{2} \mathbf{E}(t) \quad (4.9.62a)$$

$$\frac{\partial}{\partial t} \mathbf{M}_p(t) + \nu_{h,p} \mathbf{M}_p(t) = \frac{\mu_0 \omega_{h,p}^2}{2} \mathbf{H}(t). \quad (4.9.62b)$$

Discretizing (4.9.46) using central difference approximation, the update coefficients in (4.9.7) and (4.9.8) is found to be

$$k_{1p} = \frac{1 - \frac{\nu_{e,p} \Delta t}{4}}{1 + \frac{\nu_{e,p} \Delta t}{4}}; \quad k_{2p} = \frac{\epsilon_0 \omega_{e,p}^2 \Delta t / 8}{1 + \frac{\nu_{e,p} \Delta t}{4}}; \quad k_{3p} = k_{2p}; \quad (4.9.63a)$$

$$l_{1p} = \frac{1 - \frac{\nu_{h,p} \Delta t}{4}}{1 + \frac{\nu_{h,p} \Delta t}{4}}; \quad l_{2p} = \frac{\mu_0 \omega_{h,p}^2 \Delta t / 8}{1 + \frac{\nu_{h,p} \Delta t}{4}}; \quad l_{3p} = l_{2p}. \quad (4.9.63b)$$

4.10 Conclusions

Lyapunov and matrix norm stability analysis has been applied on various ADI-FDTD schemes for doubly lossy media. Among the schemes considered are averaging, forward-backward, backward-forward, forward-forward, exponential time differencing and backward-backward. From the analysis, it has been found that all schemes except backward-backward scheme are unconditionally stable. For backward-backward scheme, the condition for stability has been determined.

The unified efficient FADI-FDTD schemes for doubly lossy media has been pre-

sented. The schemes presented include averaging, forward-forward, forward-backward and novel exponential time differencing schemes. Unifications of these schemes in both conventional and efficient fundamental forms of source-incorporated ADI-FDTD have been provided. In the latter, they have been formulated in the simplest, most concise, most efficient, and most fundamental form of ADI-FDTD. The unified update equations and implementation of the efficient FADI-FDTD schemes have been provided. Such efficient fundamental schemes have substantially less RHS update coefficients and field variables compared to the conventional ADI-FDTD schemes. Thus, they feature higher efficiency with reduced memory indexing and arithmetic operations. Other aspects such as field and parameter memory arrays, PEC and PMC implementations have been discussed. Numerical results in the realm of CPU time saving, asymmetry and numerical errors as well as SAR of human skin have been presented. The generalized formulation of FADI-FDTD method for dispersive media has also been provided. It is efficient, robust and applicable to Debye, Lorentz, Drude and general complex conjugate pole-residue pair models.

Chapter 5

Applications of FADI-FDTD Method for Lossy and Dispersive Media

5.1 Introduction

Previous chapters have presented various aspects of FDTD methods for lossy and dispersive media, comprising mathematical analysis, concise formulations as well implementations. In this chapter, we shall present the applications of FADI-FDTD method for lossy and dispersive media mainly in the areas of electromagnetic compatibility, bioelectromagnetics, as well as photonics. Firstly, the modeling of reverberation chamber in mode-stirred operation is presented. A time variant complex relative permittivity is introduced such that the boundary conditions inside the chamber can be altered continuously, i.e., the mode-stirred operation. For application in bioelectromagnetics, the interaction of light with hemoglobin at optical frequency is presented. An accurate model based on complex conjugate pole-residue pairs is proposed to model the complex permittivity of hemoglobin at optical frequency. Besides that, the interaction of terahertz pulse with healthy skin and BCC is demonstrated, where the human skin is modeled as Debye media. For application in photonics, the characteristics of a surface plasmon waveguides with Au (gold)

and Ag (silver) metal cladding, modeled as combination of Drude-Lorentz dispersive media are analyzed. Further analysis of plasmonic waveguide grating filter is also considered.

5.2 Modeling Reverberation Chamber in Mode-Stirred Operation

The use of reverberation chamber to perform electromagnetic compatibility test has attracted much interests of late. Reverberation chamber is essentially an enclosed cavity with several stirrers to alter the boundary conditions so as to achieve field uniformity inside the enclosed area. There are generally two types of operations in which the reverberation chamber is used to perform electromagnetic compatibility test, namely, mode-tuned and mode-stirred operations. In mode-tuned operation, the field measurements are made at each discrete positions of the stirrer, i.e., the stirrer is moved to a new position and the measurements are repeated for every new position. On the other hand, in mode-stirred operation, field measurements are made continuously as the stirrer switches position, and the average measurements are taken over a duration of time.

The FDTD method had been used in the past to model the reverberation chamber [126–129]. They mostly used Yee’s explicit FDTD method which is subjected to the CFL condition. Furthermore, the simulations are catered for mode-tuned operation whereby the current source and fields inside the chamber are initialized to zero for every new discrete position of the stirrer. In this chapter, we shall present the modeling of the reverberation chamber in a mode-stirred operation using the FADI-FDTD method, where the stirrer is rotated continuously while fields are not initialized to zero for different stirrer position. Field uniformity and the lowest usable frequency (LUF) of the chamber shall be investigated.

5.2.1 Time Variant Conductivity Model for Reverberation Chamber in Mode-Stirred Operation

In mode-stirred operation, the boundary conditions inside the reverberation chamber are altered over time so that different modes can be generated to achieve field uniformity. The changing in boundary conditions at certain positions inside the reverberation chamber can be achieved by introducing the time variant conductivity in the Maxwell's equation as

$$\nabla \times \mathbf{H}(t) = \epsilon_0 \epsilon_r \frac{\partial}{\partial t} \mathbf{E}(t) + \sigma(t) \mathbf{E}(t) \quad (5.2.1)$$

where t is time. Note that the lossy media now has a time variant conductivity $\sigma(t)$. Using (5.2.1), we can model the changing boundary conditions inside the reverberation chamber by introducing a suitable time variant conductivity profile. Since the FADI-FDTD method is a time domain based method, the time variant conductivity model can be realized conveniently.

5.2.2 Numerical Results

We shall now demonstrate the use of FADI-FDTD in modeling reverberation chamber in mode-stirred operation. Consider a reverberation with dimensions along the x (width), y (length) and z (height) directions of 8.5 m, 12.5 m and 2 m, respectively. The fundamental resonant frequency of the cavity is around 20 MHz. The stirring effect is realized by introducing a time variant lossy media resembling a rotation of a stirrer along z -axis. The conductivity of the stirrer is set as 100. The centre of rotation is chosen at position (4.25 m, 9 m, 1 m) and the stirrer has length, width and thickness of 2.7 m, 2 m and 0.05 m, respectively.

The source excitation is chosen to be a point current source with equal strength in x , y and z components located at position (4.25 m, 0.9 m, 1 m). The source is a

Figure 5.1: Magnitude of electric field components at 200 MHz along a line.

modulated Gaussian pulse with frequency content of 80 MHz to 200 MHz. In this numerical experiment, we shall adopt a nonuniform cell size along x and y -directions. The cavity is generally meshed by a coarser cell size ($\Delta x = \Delta y = \Delta z$) of 0.1 m, which resolves around 1/15 times the wavelength at highest frequency 200 MHz. To achieve a higher accuracy for the rotation of the stirrer, the area of rotation of the stirrer is meshed at a finer cell size. The area enclosed between $x = 2.9$ m, $x = 5.6$ m, $y = 7.6$ m, $y = 10.3$ m are meshed with a cell size ($\Delta x = \Delta y$) of half the size of the coarser mesh at 0.05 m. Δz is preserved at 0.1 m throughout the whole computational domain. The time step is set at CFLN=3.5 (with respect to the finer mesh). The time variant lossy media is changed such that for every 200 time steps, the stirrer is rotated one degree. The simulation is terminated after the stirrer has made 180 degrees.

In this numerical example we shall investigate the field uniformity and LUF of the chamber. Individual time domain electric field components are recorded along a line parallel to x -axis and cutting through the centre of the chamber. A suitable windowing function such as Blackman Harris window is applied with a window length of 4000 time samples and time offset of 2000 time samples for the subsequent window.

Figure 5.2: Same as Fig. 5.1, but for reverberation chamber with stationary stirrer.

This gives rise to 17 independent time ensembles. Discrete Fourier Transform is applied to obtain the frequency spectrum from 80 MHz to 200 MHz and the average amplitude from these ensembles is taken. Fig. 5.1 plots the magnitude of electric field components along the above said line at 200 MHz. Field uniformity can be observed as the magnitude of the field components does not fluctuate too much. For comparison, Fig. 5.2 plots the electric field components along the same line at 200 MHz for a reverberation with stationary stirrer. It can now be seen that the magnitude of the field components do fluctuate more and the field uniformity has deteriorated. This is because without the stirring effect, standing waves are formed inside the chamber which does not exhibit any field uniformity.

We proceed to quantify the fluctuation of the fields and define the standard deviation, $stdev$ as

$$stdev = \sqrt{\frac{\sum_i (E_i - \langle E \rangle)^2}{n}} \quad (5.2.2)$$

where n is the number of ensembles and $\langle E \rangle$ is the mean value of the average amplitude of electric field components over different positions. The standard deviation

Figure 5.3: Standard deviation (in dB) of electric field components with respect to frequency.

can be expressed in dB as

$$stdev(dB) = 20 \log_{10} \left(\frac{stdev + \langle E \rangle}{\langle E \rangle} \right) \quad (5.2.3)$$

Fig. 5.3 plots the standard deviation (in dB) of E_x , E_y and E_z with respect to frequency. The strength of FADI-FDTD is evident here as the standard deviation of the whole frequency spectrum can be obtained in only single simulation. It is first observed that the standard deviation increases as the frequency decreases. This is commonly due to the fact that the mode densities of the chamber in the lower frequency region are not sufficient to sustain the field uniformity. The International Electrotechnical Commission (IEC) has specified that the standard deviation should be within 3 dB [130]. Thus, we can find the LUF of the chamber from Fig. 5.3 to be around 130 MHz, in which the standard deviation has exceeded the permissible 3 dB. In other words, the chamber should provide sufficient field uniformity for performing electromagnetic compatibility test above 130 MHz. For comparison, Fig. 5.4 plots the standard deviation (in dB) of E_x , E_y and E_z with respect to frequency for a reverberation chamber with stationary stirrer. We can observe now

Figure 5.4: Same as Fig. 5.3, but for reverberation chamber with stationary stirrer.

that the standard deviation is generally higher than 3 dB and has exceeded the IEC requirement for field uniformity.

5.3 Modeling Hemoglobin at Optical Frequency Using FADI-FDTD Method

The information on optical properties of human blood is crucial for many medical applications. In particular, the hemoglobin in red blood cells plays an important role by transporting oxygen throughout the human body. Past literatures have successfully determined the molar extinction coefficient [131–137] of hemoglobin at optical frequency. The real part of its complex refractive index has also been found using transmittance and reflectance measurements [138–140]. With such knowledge on the complex refractive index, a better understanding of the interaction of light with the biological media is greatly desired. Up to date, there is still a lack of appropriate complex permittivity models for biological media (in this case, hemoglobin) at optical frequency. In this section, we seek to address the aforementioned problems and bridge the necessary gaps. First, we propose a model based on complex con-

jugate pole-residue pairs to describe the electrical behaviour of hemoglobin, where it is fitted against the complex refractive index data. Once an accurate model is found, the FADI-FDTD method with incorporated complex conjugate pole-residue pairs model can be used. Some numerical examples are provided to validate the proposed method and to demonstrate some electromagnetic wave interactions with human blood at optical frequency.

5.3.1 Complex Relative Permittivity Model for Hemoglobin

We first denote the wavelength dependent complex refractive index of hemoglobin as

$$n(\lambda) = n_r(\lambda) - jn_k(\lambda) \quad (5.3.1)$$

where n_r is the real part of the refractive index and n_k is known as the extinction coefficient which is related to the absorption coefficient, μ_a of the medium by

$$n_k = \frac{\mu_a \lambda}{4\pi} \quad (5.3.2)$$

with λ being the free space wavelength. n_k is always positive to yield negative imaginary part in (5.3.1) for losses or absorption in the media.

We make use of the tabulated molar extinction coefficient, e , data in [135]. The absorption coefficient of various hemoglobin concentrations can be obtained from the molar extinction coefficient by means of the following relation:

$$\mu_a = \ln(10) \times e \times \frac{C}{64500} \quad (5.3.3)$$

where C is the hemoglobin concentration in g/L. Note that e has the unit of $\text{L mol}^{-1} \text{ cm}^{-1}$ or $\text{M}^{-1} \text{ cm}^{-1}$ and 64500 is the gram molecular weight of hemoglobin in g/mol. Once the absorption coefficient is obtained, the imaginary part of the

Figure 5.5: (a) Real part of complex refractive index, n_r and (b) extinction coefficient, n_k versus wavelength, λ for different hemoglobin concentrations. Both n_r and n_k increase with higher hemoglobin concentration across all wavelengths.

complex refractive index can be extracted through (5.3.2). On the other hand, the real part of the complex refractive index of hemoglobin at optical frequency has been determined and it is found to be related to the real part of the complex refractive index of water through a model function proposed in [140] as

$$n_r = n_{wr}(\beta c + 1) \quad (5.3.4)$$

where n_{wr} is the real part of complex refractive index of water and c is the hemoglobin concentration in g/dL (1 dL = 0.1 L). β is the specific refractive increment which is also wavelength dependent and tabulated in [140].

Therefore, using (5.3.3) and (5.3.4), the complex refractive index of hemoglobin at optical frequency can be extracted for various concentrations conveniently. Fig. 5.5 plots the (a) real part of complex refractive index, n_r and (b) extinction coefficient, n_k , respectively, versus wavelength, λ for various hemoglobin concentrations. It can be seen that n_r increases with higher hemoglobin concentration across all wavelengths. The same also holds true for n_k , which indicates that higher hemoglobin

concentration results in higher absorption (more loss). Another point to note is that when the hemoglobin concentration is at 0 g/dL, its n_r corresponds to that of water [141]. At this 0 g/dL concentration the n_k value is also reduced to zero. This is based on the fact that water has a “transparency window” at the visible light and near infrared region, in which it has negligible absorption or losses.

In electromagnetic analysis, we are more interested in the complex relative permittivity rather than the refractive index. The complex relative permittivity is related to the refractive index by

$$\begin{aligned}\epsilon(\omega) &= n(\omega)^2 \\ &= n_r(\omega)^2 - n_k(\omega)^2 - j2n_r(\omega)n_k(\omega)\end{aligned}\quad (5.3.5)$$

where the wavelength dependence has been changed into angular frequency, $\omega = 2\pi f$ dependence. The complex relative permittivity values at various frequencies (wavelengths) can then be extracted using (5.3.5) from the values of n_r and n_k earlier. We now propose a complex relative permittivity model for hemoglobin. It can be described based on complex conjugate pole-residue pairs as follows:

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \left(\frac{r_p}{j\omega - a_p} + \frac{r_p^*}{j\omega - a_p^*} \right) \quad (5.3.6)$$

The model based on complex conjugate pole-residue pairs in (5.3.6) is then fitted against the complex relative permittivity data extracted from (5.3.5) using the methodology detailed in [142] to obtain the values of ϵ_∞ , a_p and r_p . The values are fitted within the frequency range of 300 THz to 1200 THz (250 nm-1000 nm wavelength). In practical medical applications we are often interested in only two hemoglobin concentrations. The first one is the hemoglobin concentration in erythrocytes (red blood cells), which is also commonly known as mean corpuscular hemoglobin concentration (MCHC). Typical MCHC value for a healthy adult is

Table 5.1: Fitted values of a_p , r_p and ϵ_∞ for hemoglobin concentration of 15 g/dL

p	a_p	r_p
1	$-3.1751 \times 10^{14} + j2.4717 \times 10^{15}$	$-2.0191 \times 10^{10} + j1.6882 \times 10^{10}$
2	$-7.1750 \times 10^{13} + j3.2611 \times 10^{15}$	$1.1223 \times 10^{11} - j2.0688 \times 10^{11}$
3	$-3.6183 \times 10^{13} + j3.4679 \times 10^{15}$	$3.6477 \times 10^{10} - j9.6911 \times 10^{10}$
4	$-1.4538 \times 10^{14} + j4.5108 \times 10^{15}$	$7.1508 \times 10^{11} - j3.6455 \times 10^{12}$
5	$-1.5535 \times 10^{14} + j5.3385 \times 10^{15}$	$2.0872 \times 10^{11} - j2.2396 \times 10^{11}$
6	$-3.2153 \times 10^{13} + j9.5959 \times 10^{15}$	$-4.2183 \times 10^{12} - j3.9864 \times 10^{14}$

$$\epsilon_\infty = 1.7844$$

Table 5.2: Fitted values of a_p , r_p and ϵ_∞ for hemoglobin concentration of 33 g/dL

p	a_p	r_p
1	$-3.1751 \times 10^{14} + j2.4717 \times 10^{15}$	$-3.8401 \times 10^{10} + j5.8207 \times 10^{10}$
2	$-7.1750 \times 10^{13} + j3.2611 \times 10^{15}$	$2.8608 \times 10^{11} - j5.0495 \times 10^{11}$
3	$-3.6183 \times 10^{13} + j3.4679 \times 10^{15}$	$1.0080 \times 10^{11} - j2.2246 \times 10^{11}$
4	$-1.4538 \times 10^{14} + j4.5108 \times 10^{15}$	$1.6344 \times 10^{12} - j8.0730 \times 10^{12}$
5	$-1.5535 \times 10^{14} + j5.3385 \times 10^{15}$	$3.6171 \times 10^{11} - j5.2711 \times 10^{11}$
6	$-3.2153 \times 10^{13} + j9.5959 \times 10^{15}$	$-1.4155 \times 10^{13} - j4.5947 \times 10^{14}$

$$\epsilon_\infty = 1.8994$$

around 33 g/dL. The second one is the overall hemoglobin concentration in human blood, which consists of not only erythrocytes, but also leukocytes (white blood cells), thrombocytes (platelets) and plasma. The overall hemoglobin concentration for a healthy adult is around 15 g/dL, and this corresponds to hematocrit (which is the proportion of blood volume that is occupied by red blood cells) of around 45 percent. It is found that using 6 pairs (order 12) of complex conjugate pole and residue pairs can sufficiently fit the experimental data. The values of ϵ_∞ , a_p and r_p for hemoglobin concentrations of 15 g/dL and 33 g/dL are provided in Tables 5.1 and 5.2, respectively. Since all hemoglobin concentrations have rather the same trends

Figure 5.6: (a) Real part, ϵ_{rr} and (b) imaginary part, ϵ_{ri} of complex relative permittivity versus wavelength, λ : model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL. A good fit is observed between our proposed model and experimental data across all wavelengths.

of complex relative permittivity or complex refractive index, we assume that they all share the same poles a_p . That is, once the poles are identified for one hemoglobin concentration, they can be reused as poles of other hemoglobin concentrations. Only the new values of residues are calculated to avoid tedious searching of new poles.

Using the values provided in Tables 5.1 and 5.2, we plot the real and imaginary part of the fitted model based on complex conjugate pole-residue pairs and compare them with the experimental data obtained in the previous subsection. Fig. 5.6 plots the (a) real and (b) imaginary parts of the complex relative permittivity versus wavelength for both our model and experimental data. Fig. 5.7 plots the (a) real and (b) imaginary parts of the complex refractive index versus wavelength for both our model and experimental data. The absorption coefficient is then plotted in Fig. 5.8. It is evident that our model in (5.3.6), along with the values given in Tables 5.1 and 5.2, provide a good fit to the experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL. The proposed model is thus expected to

Figure 5.7: (a) Real part, n_r and (b) imaginary part, n_i of complex refractive index versus wavelength, λ : model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL.

describe the electromagnetic behaviour of hemoglobin accurately in the wavelength regions of 250 nm to 1000 nm.

5.3.2 Numerical Results

Transmission and Reflection Coefficients

To demonstrate the accuracy of our hemoglobin model in the FADI-FDTD method, we first compute the transmission and reflection coefficients of a half space human blood numerically. A modulated Gaussian pulse is launched from free space and upon hitting the human blood interface, undergoes transmission and reflection. The modulated Gaussian pulse has a bandwidth of 1500 THz around centre frequency of 750 THz, thus covering the entire frequency spectrum of the human blood model (300 THz to 1200 THz). The model of 15 g/dL hemoglobin concentration (Table 5.1) is used. Cell size is set at 3.125 nm which corresponds to CPW of around 50 for the shortest wavelength in the human blood (wavelength in human blood, $\lambda \approx \lambda_0/1.5$,

Figure 5.8: Absorption coefficient, μ_a versus wavelength, λ : model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL.

where λ_0 is the wavelength in free space. The shortest wavelength considered in free space is 250 nm). The time step Δt is always specified as CFLN, which is relative to the CFL time step limit in the Yee's explicit FDTD method, i.e. $CFLN = \Delta t / \Delta t_{CFL}$ where Δt_{CFL} is the maximum allowed time step of Yee's explicit FDTD.

The transmission and reflection coefficients (in frequency domain) can be obtained numerically by taking the ratio of the discrete Fourier transform of the transmitted and reflected wave, respectively to the discrete Fourier transform of the incident wave. The numerical experiment is run for various CFLNs to validate the accuracy of the hemoglobin model under different time steps. Fig. 5.9 graphs the magnitude of the computed (a) transmission and (b) reflection coefficients, respectively versus frequency for various CFLNs. They are compared against the reference transmission and reflection coefficients of our analytical hemoglobin model. Also shown in the figures are the transmission and reflection coefficients computed using the Yee's explicit FDTD method. Since the Yee's explicit FDTD method is not unconditionally stable, it is run at its maximum time step limit of CFLN=1. Any time step larger than that will render the algorithm unstable. The FADI-FDTD method is

Figure 5.9: Magnitude of (a) transmission and (b) reflection coefficients versus frequency for various CFLNs.

unconditionally stable, and therefore we can see that CFLN beyond 1 still yield considerably accurate results. Nevertheless, the accuracy of the FADI-FDTD method deteriorates as the CFLN increases, especially towards higher frequency region. This is because as the frequency increases, higher CFLN (and thus larger time step) fails to resolve these higher frequency components sufficiently. Therefore, larger chosen time step increases the simulation speed, but at the expense of sacrificing a certain degree of accuracy. Based on these results, we can see that the chosen time step in FADI-FDTD is always a compromise between efficiency and accuracy.

Specific Absorption Rate (SAR)

SAR is an important measure for biological media exposed to electromagnetic radiation, which describes the electromagnetic energy absorption rate. It is defined as

$$SAR = \frac{s_l}{\rho} \quad (5.3.7)$$

where s_l is the power loss density in W/m^3 and ρ is the density of the biological media in kg/m^3 , which gives the SAR the overall unit of W/kg . In most of the previous SAR analysis literatures [143–146], the power loss density is usually computed using

$$s_l = \frac{1}{2} \sigma |\tilde{\mathbf{E}}|^2 \quad (5.3.8)$$

where $\tilde{\mathbf{E}}$ is the phasor form (without time dependence) of the electric field components. In time domain methods, such as the FDTD methods, the significant benefit is such that a narrow pulse can be injected to provide a wide range of frequency points using only a single run of simulation. In this case, $\tilde{\mathbf{E}}$ can be the Fourier transform of the recorded electric field components, which gives us the information across a range of frequency resulted from illumination by any sinusoidal (monochromatic) source. This however, can only be performed if the medium of interest is modeled as the simplest case of conductive media, described by only a single conductivity value across the frequency range of interest. This is usually not the case in most biological media, such as the human blood described in this section, where the conductivity changes with frequency. To use (5.3.8), the simulation has to be carried out point by point across the frequency range of interest using sinusoidal excitation, along with the corresponding conductivity values at different frequency. The advantage of FDTD method is thus not being exploited fully.

Since we have successfully modeled human blood across a range of optical frequency based on complex conjugate pole-residue pairs along with its implementation using the FADI-FDTD method, the power loss density formula in (5.3.8) can be modified to better suit our scenario. For a dispersive medium which has a complex permittivity of $\epsilon = \epsilon' - j\epsilon''$, where ϵ' and ϵ'' are the real and negative imaginary (dissipative) parts, respectively, the power loss density can be found using [147, 148]

$$s_l = \frac{1}{2} \omega \epsilon'' |\tilde{\mathbf{E}}|^2. \quad (5.3.9)$$

Note that for conductive media with single conductivity value, $\epsilon'' = \sigma/\omega$ and (5.3.9) conforms to (5.3.8), which is considered as a special case for simplest conductive media. Hence, (5.3.9) is the generalization of power loss density for dispersive media. Using (5.3.9), we are now able to obtain the information across a range of frequency with only a single run of simulation, which is highly efficient.

In the following numerical example, we consider a capillary (blood vessel) in our body, and has a typical diameter of 8 μm . The straight long capillary is oriented along z -direction and is surrounded by tissue, which is assumed to be made up of mostly water and thus, having similar dielectric properties of water. Since the water has negligible absorption in the visible light and near infrared region, the refractive index is taken as a constant value of 1.33. Both models of 15 g/dL and 33 g/dL hemoglobin concentrations are applied to the capillary. The cell size is chosen as 11.1 nm which corresponds to CPW of 15 at shortest wavelength in the human blood and the time step is chosen at CFLN=4. A z -directed line current source of the same modulated Gaussian pulse as the previous subsection illuminates upon the capillary, exciting the frequency contents from 300 THz to 1200 THz. The perfectly matched layer [125] terminates the computational boundaries.

At steady state, the SAR values at different locations of the capillary are computed using (5.3.7) and (5.3.9) and the density, ρ of the human blood is 1060 kg/m³ [146]. The SAR is computed at frequencies of 440 THz, 550 THz and 720 THz. These frequencies correspond to free space wavelengths of 680 nm, 545 nm and 417 nm. Referring to Fig. 5.8, wavelength at 417 nm is where the highest absorption peak occurs, followed by 545 nm. The lowest absorption occurs at 680 nm. Figs. 5.10, 5.11 and 5.12 illustrate the SAR values (in W/kg) at different locations of the capillary at 440 THz, 550 THz and 720 THz, respectively. All the SAR values are plotted in logarithmic scale ($\log_{10} SAR$). All figures (a) refer to hemoglobin concentration of

Figure 5.10: SAR (in logarithmic scale) at different locations of capillary at 440 THz (680 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.

15 g/dL while figures (b) refer to hemoglobin concentration of 33 g/dL. The SAR values at each location have been scaled to correspond to incident power density $S = \frac{1}{2} \text{Re}(\tilde{\mathbf{E}} \times \tilde{\mathbf{H}}^*)$ of 1 mW/m² in free space. Note that the source illuminates from the left to right of the figures. We first notice that frequency at 720 THz (417 nm), c.f. Fig. 5.12 gives rise to the highest SAR values, followed by 550 THz (545 nm), c.f. Fig. 5.11 and 440 THz (680 nm), c.f. Fig. 5.10. This is in consistent with the absorption coefficient profile in Fig. 5.8. Another interesting observation is that at only 720 THz (417 nm), the SAR in the capillary shows a descending trend from the left to right along the wave travelling direction, while other frequencies show rather uniform SAR across the whole capillary region. This indicates that at the absorption peak of 720 THz (417 nm), the bulk of the power is absorbed near the left side, which results in lesser power penetration across the capillary. On the other hand, the absorbed power is well distributed across the whole region of the capillary at other frequencies due to weaker absorption. The standing wave effect may be attributed to the closed volume of the capillary. At the same time, it is observed

Figure 5.11: SAR (in logarithmic scale) at different locations of capillary at 550 THz (545 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.

Table 5.3: Maximum and Average SAR values computed using FADI-FDTD and explicit FDTD at hemoglobin concentration of 15 g/dL

Frequency/Wavelength	FADI-FDTD		explicit FDTD	
	SAR max (W/kg)	SAR avg (W/kg)	SAR max (W/kg)	SAR avg (W/kg)
440 THz (680 nm)	2.4870×10^{-4}	1.5662×10^{-4}	2.5134×10^{-4}	1.5659×10^{-4}
550 THz (545 nm)	0.0438	0.0243	0.0445	0.0247
720 THz (417 nm)	0.2783	0.0969	0.2758	0.0964

that capillary with hemoglobin concentration of 33 g/dL generally exhibits higher SAR values across all frequencies. This concentration represents that of only the red blood cells, and could possibly model blood clot inside a capillary, which is formed as a result of entrapment of red blood cells [149]. Thus, the SAR calculation reveals that blood clot has a higher absorption compared to normal blood, which could be useful for medical applications and diagnostics.

We have also performed similar numerical example using the Yee's explicit FDTD method. Tables 5.3 and 5.4 show the maximum and average SAR of the capil-

Figure 5.12: SAR (in logarithmic scale) at different locations of capillary at 720 THz (417 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.

Table 5.4: Maximum and Average SAR values computed using FADI-FDTD and explicit FDTD at hemoglobin concentration of 33 g/dL

Frequency/Wavelength	FADI-FDTD		explicit FDTD	
	SAR max (W/kg)	SAR avg (W/kg)	SAR max (W/kg)	SAR avg (W/kg)
440 THz (680 nm)	0.0012	4.5712×10^{-4}	0.0012	4.5704×10^{-4}
550 THz (545 nm)	0.1574	0.0491	0.1654	0.0510
720 THz (417 nm)	0.6021	0.0914	0.5973	0.0906

lary computed using the FADI-FDTD method and Yee's explicit FDTD method at hemoglobin concentrations of 15 g/dL and 33 g/dL. It can be seen that the calculated SAR values are quite close to each other. This shows that using the FADI-FDTD method at CFLN=4 does not suffer too much from accuracy deficiency. It is also found that the simulation time incurred by the FADI-FDTD method at CFLN=4 in Matlab codes is around 3 times faster than that of the Yee's explicit FDTD method. These further show that while maintaining accuracy, the FADI-FDTD method is promising in achieving higher efficiency for modeling biological media.

5.4 Modeling the Interaction of Terahertz Pulse with Healthy Skin and Basal Cell Carcinoma (BCC) Using FADI-FDTD Method

Terahertz radiation typically occupies the electromagnetic spectrum between 0.1 THz to 10 THz ($1 \text{ THz} = 10^{12} \text{ Hz}$), and has widespread biomedical application involving the interaction of terahertz pulse with biological media [150–153]. Among them, terahertz radiation has been used successfully as a noninvasive imaging technique for detection of human skin cancer [154–159], in particular, the BCC. The healthy human skin and BCC have shown different response under the radiation of terahertz pulse and it is possible for terahertz pulse radiation to differentiate between healthy skin and BCC in outlining the tumour margin prior to surgery, such as the Mohs micrographic surgery (MMS). All these further necessitate a better understanding of the interaction of terahertz pulse with healthy skin and BCC.

Some numerical examples involving the interaction of terahertz pulse with human skin in only 1-D system have been shown in [160] and [161] using Yee's explicit FDTD method. The modeling in this section is based on the unconditionally stable FADI-FDTD method. The full three dimensional FADI-FDTD will be employed to model the terahertz pulse interaction with healthy skin and BCC. The healthy skin and BCC are both modeled as Debye dispersive media and the model is then incorporated into our FADI-FDTD method. Numerical experiments on delineating the BCC margin from healthy skin will be demonstrated based on both reflected terahertz pulse. It will be shown that terahertz pulse radiation can indeed be used for successful detection of BCC in medical application.

Table 5.5: Debye parameters for healthy skin and BCC in terahertz region

	ϵ_∞	$\Delta\epsilon_1$	$\Delta\epsilon_2$	τ_1/ps	τ_2/ps
healthy skin	2.58	10.54	1.58	1.45	0.0611
BCC	2.65	13.37	1.58	1.55	0.0614

Figure 5.13: (a) Real part of complex refractive index, n_r and (b) absorption coefficient, μ_a versus frequency for healthy skin and BCC. BCC generally has higher n_r and μ_a than healthy skin throughout the terahertz region.

5.4.1 Complex Relative Permittivity Model for Human Skin

It has been shown in [161] that the complex permittivity for both healthy skin and BCC in the terahertz region can be modeled using the Debye dispersive media. The general complex permittivity model of a Debye dispersive medium is described by

$$\epsilon(\omega) = \epsilon_\infty + \sum_p \frac{\Delta\epsilon_p}{1 + j\omega\tau_p} \quad (5.4.1)$$

It is found that two Debye poles are sufficient to describe the complex permittivity of healthy skin and BCC in the terahertz region of 0.2 THz to 2 THz [161] and their Debye parameters are tabulated in Table 5.5. Fig. 5.13 shows the (a) real part of complex refractive index, n_r and (b) absorption coefficient, μ_a versus frequency for

healthy skin and BCC. We can see that BCC generally has higher n_r and μ_a than healthy skin throughout the terahertz region. It is anticipated that with a difference in both n_r and μ_a between healthy skin and BCC, they will exhibit different response under terahertz pulse radiation. The different terahertz pulse radiation response shall be demonstrated in the subsequent sections.

5.4.2 Reflected terahertz pulse

We now demonstrate the use of FADI-FDTD in the simulation of human skin *ex vivo*. Half-spaced healthy skin and BCC are considered separately and they are subjected to illumination by Gaussian pulse with frequency content of up to 2 THz. Cell size is set at $1.8 \mu\text{m}$ which resolves around $1/40$ times the wavelength in the human skin at 2 THz. The time step Δt is specified as CFLN. In this case, we choose CFLN=10. The healthy skin and BCC both have Debye parameters adopted from Table 5.5. The terahertz pulse is incident upon the human skin from a quartz medium having a constant relative permittivity of 4.5 [161]. The quartz-skin interface is considered because the skin samples are placed between sample holders made of quartz during imaging [155]. The terahertz pulse, upon incident at the surface of the human skin, undergoes reflection. The reflected terahertz pulse from healthy skin and BCC is observed and recorded.

After the reflected terahertz pulse is recorded, signal post-processing procedure similar to that in [155] is applied. The reflected terahertz pulse is Fourier transformed into frequency domain $\tilde{E}^r(f)$, and divided by $\tilde{E}^{air}(f)$, obtained from the reflected terahertz pulse off a quartz-air interface. Subsequently, windowing transfer function or filter is multiplied to it. The post-processed electric field in frequency domain $\tilde{E}(f)$ is given by

$$\tilde{E}(f) = \frac{\tilde{E}^r(f)}{\tilde{E}^{air}(f)} \times \tilde{W}(f). \quad (5.4.2)$$

Figure 5.14: Post-processed terahertz pulse from healthy skin and BCC computed using FADI-FDTD and explicit FDTD. The reflected terahertz pulse from BCC has a larger amplitude than the reflected terahertz pulse from healthy skin.

Finally inverse Fourier transform is applied to $\tilde{E}(f)$ to obtain the final post-processed electric field in time domain as

$$E(t) = \mathcal{F}^{-1} \left\{ \tilde{E}(f) \right\}. \quad (5.4.3)$$

Note that the post-processing procedure is applied so that the impulse response of the human skin can be obtained.

Fig. 5.14 shows the post-processed terahertz pulse (electric field) from healthy skin and BCC. In this figure, the filter chosen is a Gaussian function with frequency content of up to 2 THz. We first observe that the post-processed electric field is negative. In the quartz-skin interface, the terahertz pulse is reflected off human skin which has generally higher refractive index compared to the incident medium quartz. On the other hand, in the quartz-air interface, the terahertz pulse is reflected off air which has lower refractive index compared to the incident medium quartz. This results in opposite phase between these two reflected terahertz pulse, and hence negative post-processed electric field. It can be seen that the reflected terahertz pulse

Figure 5.15: Illustration of the numerical scanning process and geometrical setup of human skin model.

from BCC has a larger amplitude (more negative) than the reflected terahertz pulse from healthy skin. Since the difference in the refractive index between BCC and quartz is higher than that of healthy skin and quartz (c.f. Fig. 5.13), the terahertz pulse is reflected more from BCC compared to that of healthy skin. The simulation obtained using the Yee's explicit FDTD method is also provided for comparison. It is observed that at CFLN=10 (time step 10 times larger), the FADI-FDTD and Yee's explicit FDTD methods are in excellent agreement with each other. Furthermore, it is also in agreement with the result shown in past literature, c.f. Figure 3 in [161]. Hence, it can be found that the reflected terahertz pulse can be used to distinguish between a healthy skin and BCC.

5.4.3 BCC detection based on reflected terahertz pulse

With such a difference in reflected terahertz pulse between healthy skin and BCC, we next demonstrate numerical examples of BCC detection based on terahertz pulse

illumination using the FADI-FDTD method. The numerical scanning process using the terahertz pulse illumination and geometrical setup of the human skin model are shown in Fig. 5.15. Let the depth of the skin oriented along the x -direction. A z -directed line current source, s_{ez} is oriented parallel to the skin surface and it is scanned along the skin surface in the y -direction. The scanning area is chosen to be $420 \mu\text{m} \times 420 \mu\text{m}$. While the line current source is scanned along the skin surface, the reflected terahertz pulse from each and every point of the skin surface is also collected at the same time. The scanning proceeds until the entire skin surface area is completed. After that, the post-processing procedure as detailed before is applied. The filter is now chosen to be modulated Gaussian function with frequency content of 0.2 to 2 THz. It is more appropriate compared to the Gaussian function in previous subsection as the two-pole Debye media used to describe the human skin is within terahertz range of 0.2 to 2 THz. Based on the post-processed reflected terahertz pulse of each point, the post-processed peak-to-peak of z -directed electric field, E_{zpp} is extracted.

The procedure is repeated with the z -directed line current source replaced by a y -directed line current source, s_{ey} and it is now scanned along the skin surface in the z -direction. Now, the post-processed peak-to-peak of y -directed electric field, E_{ypp} is extracted. Using the results of the reflected terahertz pulse from two line current sources (z -directed and y -directed), we obtain the overall post-processed peak-to-peak electric field, E_{pp} by

$$E_{pp} = \frac{1}{2}(E_{zpp} + E_{ypp}). \quad (5.4.4)$$

Note that we take the average value of the post-processed peak-to-peak terahertz pulse obtained by these two line current sources. By doing so, the characteristics of the reflected pulse from two orthogonal line current sources can be taken into consideration. Furthermore, by using two orthogonal line current sources, only two

“sweeps” are needed in two orthogonal directions to complete the scanning process for the entire surface area of the skin. This is far more efficient than the conventional way of point by point scanning. The use of lenses for focusing the terahertz laser beam in the point by point scanning procedure is also redundant. This further simplifies the whole scanning process.

BCC originates from the basal layer of the epidermis, the top most layer of the human skin. Typically, the human epidermis has an average thickness of around 100 μm [162,163]. In our numerical scanning example, the human skin consists of a 300 μm thick healthy skin and a patch of BCC, also with thickness 300 μm encapsulated within the healthy skin. With a patch thickness of 300 μm , the BCC is assumed to infect the entire layer of epidermis, and extending into the dermis layer, which is the second layer of human skin after epidermis. The patch of BCC has a circular cross sectional area with a radius of 150 μm . Looking from the top, the circular patch of BCC is surrounded by healthy skin tissue. Uniform cell size ($\Delta x = \Delta y = \Delta z$) is now set at 6 μm which resolves around 1/15 times the wavelength in the human skin at 2 THz. The time step, on the other hand is chosen at CFLN=4. The perfectly matched layer [125] is used to terminate the computational boundaries.

Fig. 5.16a plots the numerically scanned image of the overall post-processed peak-to-peak terahertz pulse, E_{pp} , normalized to the reference post-processed peak-to-peak terahertz pulse, $E_{pp(ref)}$ for the circular BCC patch. Note that this reference is obtained from a confirmed healthy skin. As such, region with value of one indicates that of a healthy skin tissue. From Fig. 5.16a, the BCC patch with circular cross sectional area of radius 150 μm can be clearly seen and E_{pp} exhibited by the BCC is around 10 percent more than that of the surrounding healthy skin tissue. To consider different shape pattern of the BCC cross sectional area, the BCC patch of circular cross sectional area is replaced with BCC patch of elliptic cross sectional

Figure 5.16: Numerically scanned images of the normalized overall post-processed peak-to-peak terahertz pulse, E_{pp} for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area. Region with value of one indicates that of a healthy skin tissue.

area. The major and minor semi-axes of the ellipse are oriented along z and y axes respectively, and their respective lengths are $180 \mu\text{m}$ and $120 \mu\text{m}$. On top of that, the BCC patch of elliptic cross sectional area is also rotated 45 degree counter-clockwise. Fig. 5.16b shows the numerically scanned image of the normalized overall reflected peak-to-peak terahertz pulse for the aforementioned BCC patch. A 45 degree counter-clockwise rotated elliptic cross sectional area with major and minor semi-axes of $180 \mu\text{m}$ and $120 \mu\text{m}$ can be clearly identified. E_{pp} of the BCC is also 10 percent more than that of the surrounding healthy skin tissue. We further consider surface roughness and structure irregularities in the human skin. Fig. 5.17 shows the numerical scanned images of the same BCC patches in Fig. 5.16, but with some roughness and irregularities randomly introduced on the surface of the human skin and edges of BCC patch. It is observed that the BCC patches are still visible, albeit some irregularities in the margin and contrast. The contrast between BCC and its surrounding healthy tissue is also approximately 10 percent.

Figure 5.17: Same as Fig. 5.16, but with roughness and irregularities on the surface of the human skin and edges of BCC patch.

Table 5.6: Variation of Debye parameters for healthy skin fitted to maximum and minimum experimental data

	ϵ_{∞}	$\Delta\epsilon_1$	$\Delta\epsilon_2$	τ_1/ps	τ_2/ps
maximum	2.62	11.96	1.58	1.5	0.0613
minimum	2.55	9.13	1.58	1.4	0.0610

Next, we consider some variability of Debye parameters in the healthy skin. Note that the Debye parameters for healthy skin in Table 5.5 is fitted based on the mean value of the data obtained from experiments in [159]. Here, we slightly vary the Debye parameters of the healthy skin to represent the maximum and the minimum values of the experimental data. Such different parameterization may be attributed to different pigmentation level in the healthy skin. The variation of Debye parameters for healthy skin is shown in Table 5.6. Fig. 5.18 shows the numerically scanned images of the normalized overall post-processed peak-to-peak terahertz pulse of elliptical BCC patch embedded within healthy skin with Debye parameters fitted to (a) maximum and (b) minimum experimental data. We can observe that for BCC patch embedded within healthy skin with Debye parameters fitted to maximum ex-

Figure 5.18: Numerically scanned images of the normalized overall post-processed peak-to-peak terahertz pulse of elliptical BCC patch embedded within healthy skin with Debye parameters fitted to (a) maximum and (b) minimum experimental data.

perimental data (c.f. Fig. 5.18a), the contrast is reduced to 5 percent compared to a contrast of 10 percent in Fig. 5.16. This is because the maximum experimental data of healthy skin is now closer to that of the BCC in terms of refractive index and absorption coefficient. On the other hand, for BCC patch embedded within healthy skin with Debye parameters fitted to minimum experimental data (c.f. Fig. 5.18b), the contrast is increased to around 18 percent compared to a contrast of 10 percent in Fig. 5.16. The minimum experimental data of healthy skin is now further away from that of the BCC. It is also mentioned in [159] that the typical signal-to-noise (SNR) ratio in the system is around 4000 (36 dB). To consider the effect of such noise in the system, we include a white Gaussian noise in the simulated reflected terahertz pulse with the same SNR. Fig. 5.19 shows the same numerical scanned images as in Fig. 5.18, but with white Gaussian noise of 36 dB SNR added to the reflected terahertz pulse. It can be seen that due to the high SNR, the contrast is not affected and the BCC patch can still be clearly identified under the influence of noise.

Figure 5.19: Same as Fig. 5.18, but with added white Gaussian noise of SNR 32 dB to the reflected terahertz pulse.

In previous numerical examples, the filter function $W(f)$ is selected as a modulated Gaussian to capture the frequency components of the reflected terahertz pulse from 0.2 to 2 THz. It is reported in [159] that a higher percentage difference of refractive index between healthy skin and BCC lies between 0.35 and 0.55 THz. Fig. 5.20 now shows the numerically scanned images of the normalized post-processed peak-to-peak terahertz pulse for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area, where the filter function is chosen to only capture the frequency components of the reflected terahertz pulse from 0.35 to 0.55 THz. It can be seen that a higher contrast of 15 percent is exhibited by the BCC patches if we were to extract the reflected terahertz pulse from 0.35 to 0.55 THz. This is consistent with the results in [159] where a higher percentage difference of refractive index between healthy skin and BCC is observed between 0.35 and 0.55 THz.

We now consider the effect of an encrusted layer on top of the BCC patch. The BCC has a thickness of 300 μm and is modeled as a two-layered medium where

Figure 5.20: Numerically scanned images of the normalized post-processed peak-to-peak terahertz pulse for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area. The filter function is chosen to only capture the frequency components of the reflected terahertz pulse from 0.35 to 0.55 THz.

the bottom layer is the BCC itself with *ex vivo* Debye parameters from Table 5.5. On top of that, there is an encrusted layer at the top with thickness of $3\text{ }\mu\text{m}$. A constant relative permittivity, ϵ_r of 3 is assumed for this encrusted layer [161]. In this numerical example we shall adopt a nonuniform cell size along the depth of the skin (x -direction). The $3\text{ }\mu\text{m}$ -thick encrusted layer is discretized by $\Delta x = 0.6\text{ }\mu\text{m}$, while the discretization for rest of the depth layer of the skin remains at $\Delta x = 6\text{ }\mu\text{m}$, i.e. the encrusted layer is discretized by cell size 10 times smaller than the rest of the depth layer. $\Delta y = \Delta z = 6\text{ }\mu\text{m}$ is preserved for the entire computational domain. Due to the unconditional stability feature of FADI-FDTD, the nonuniform cell size will further demonstrate the strengths of our FADI-FDTD since its time step is still unaffected and unrestricted by the usage of a small Δx in the encrusted layer. Fig. 5.21 plots the numerically scanned images of the normalized post-processed peak-to-peak terahertz pulse for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area.

Figure 5.21: Numerically scanned images of the normalized post-processed peak-to-peak terahertz pulse for (a) BCC patch with circular cross sectional area and (b) BCC patch with 45 degree counter-clockwise rotated elliptic cross sectional area. The BCC patches include the encrusted layer.

Table 5.7: Efficiency gain and relative root-mean-square (RMS) error of FADI-FDTD for various CFLNs

CFLN	Efficiency Gain	Relative RMS Error
4	2.44	2.65 %
10	6.10	6.42 %
15	9.15	8.34 %

Both BCC patches include a $3\text{ }\mu\text{m}$ -thick encrusted layer. It can be seen that the contrast is now as high as 40 percent between the BCC patches and the surrounding healthy skin tissue. The presence of a thin encrusted layer further increases the contrast exhibited by the BCC patches due to the fact that the difference in the refractive index between BCC (with encrusted layer) and quartz is much higher than that of healthy skin and quartz.

For comparison, the numerical example is repeated using the Yee's explicit FDTD method. Note however that the time step of the Yee's explicit FDTD method is

restricted by the CFL condition. It is determined that the time step used in the Yee's explicit FDTD method is restricted to 15 times smaller than the original time step used in FADI-FDTD, which corresponds to CFLN=15 in our FADI-FDTD method. Table 5.7 further shows the efficiency gain and relative root-mean-square (RMS) error of FADI-FDTD for various CFLNs. The efficiency gain is taken over the Yee's explicit FDTD in terms of CPU run time, while the RMS error is computed by taking the Yee's explicit FDTD as the reference solution. This table gives a clear illustration on the trade-off between accuracy and efficiency of our FADI-FDTD method. For the previous numerical example at CFLN=15, our FADI-FDTD is 9.15 times faster than the Yee's explicit FDTD method, at the expense of only 8.34 percent RMS error. For a smaller CFLN of 4, our FADI-FDTD is still 2.44 times faster than the Yee's explicit FDTD method, with higher accuracy of 2.65 percent RMS error. This implies that our FADI-FDTD method achieves a good trade-off between efficiency and accuracy.

We further consider the case of a buried BCC tumour. The BCC is now modeled as a sphere with a radius of 150 μm buried within the healthy skin. Note that the reflected peak-to-peak terahertz pulse in all the previous cases can no longer be used directly. To extract the actual reflected terahertz pulse from the buried BCC tumour, we adopt

$$E_{zb}^r = E_z^r - E_{z(ref)}^r \quad (5.4.5)$$

where E_{zb}^r is the z -directed reflected electric field from the buried BCC tumour, E_z^r is the z -directed reflected electric field recorded and $E_{z(ref)}^r$ is the reference z -directed reflected electric field, obtained from a confirmed healthy skin. Note that E_z^r consists of reflected terahertz pulse from both healthy skin and buried BCC tumour. Using (5.4.5), the desired reflected terahertz pulse from only the buried BCC tumour can be isolated. If the buried BCC tumour is not present, E_{zb}^r will be equal to zero. The

Figure 5.22: Numerically scanned images of the normalized overall post-processed peak-to-peak terahertz pulse of buried tumour, E_{bpp} with the shape of (a) sphere and (b) 45 degree counter-clockwise rotated ellipsoid. Region with value of zero indicates that of a healthy skin tissue.

post-processing in (5.4.2) and (5.4.3) are then applied to extract its peak-to-peak E_{zbpp} . Similar procedure is then applied to the y -directed electric field to obtain E_{ybpp} . Finally, the overall post-processed peak-to-peak electric field of buried BCC tumour is

$$E_{bpp} = \frac{1}{2}(E_{zbpp} + E_{ybpp}). \quad (5.4.6)$$

Fig. 5.22a shows the numerically scanned image of the normalized overall post-processed peak-to-peak terahertz pulse of the buried spherical BCC tumour E_{bpp} . In this case, region with value of zero indicates that of a healthy skin tissue (BCC tumour not present). From Fig. 5.22a, the buried BCC tumour can still be seen with E_{bpp} of approximately 10 percent more than that of the surrounding healthy tissue. For an ellipsoidal BCC tumour, its semi-principal axes oriented along x , y and z axes have the lengths of $150 \mu\text{m}$, $120 \mu\text{m}$ and $180 \mu\text{m}$, respectively. On top of that, it is also rotated 45 degree counter-clockwise along the depth axis. Depicted

in Fig. 5.22b, this buried ellipsoid can also be identified with E_{bpp} of approximately 10 percent more than that of the surrounding healthy tissue. The margin of BCC tumour is smaller compared to the previous cases due the fact that it is buried within the healthy skin.

Based on our simulations shown in Figs. 5.16, 5.21 and 5.22, it is noted that the BCC with encrusted layer exhibits higher contrast than that of BCC without encrusted layer. Thus, the presence of encrusted layer further enhances the contrast shown by the BCC. Hereby, the authors would like to point out that it is likely that the considerably good image contrast between the BCC and healthy skin as performed in the experiments in [157, 158] may not be attributed to the BCC and healthy skin alone. Rather, it is also coupled by the existence of the encrusted layer of the BCC, or perhaps other physical layers within the BCC. Furthermore, during the measurement of the complex refractive index of human skin [159] (from which the Debye parameters are extracted), the skin samples are tightly pressed between the sample holder which may have removed some of the water and intracellular fluid. As water plays an important role in terahertz region where it exhibits high absorption spectra [141], the loss of water and intracellular fluids in the skin during measurement may have caused the discrepancy between measured (and hence the Debye parameter used in numerical experiments) and actual complex refractive index of healthy skin and BCC.

5.5 Analysis of Optical Waveguide Using FADI-FDTD Method

Optical waveguide exhibiting plasmonic resonances [164–166] has attracted much interest recently as it allows guiding of light propagation in subwavelength region. The subwavelength light propagation in optical waveguide results in highly refined grids

Figure 5.23: Real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity for metal Au (gold): Drude model and experimental data.

which undesirably prolong the simulation time of the Yee's explicit FDTD method due to the CFL condition. Therefore, the FADI-FDTD method is a suitable candidate for such numerical experiment as it is very efficient and has unconditionally stable feature. In this section, we shall conduct the analysis of optical waveguide using FADI-FDTD method. The metal cladding in the optical waveguide is modeled using a combination of Drude-Lorentz dispersive model. The transmission coefficient of the optical waveguide is determined for photon energy range of 1.24 eV to 2.48 eV (wavelength 500 nm to 1000 nm). Two types of metal are considered for the cladding, which are Au (gold) and Ag (silver). On the other hand, air and SiO₂ are used separately as the material for the core.

5.5.1 Complex Relative Permittivity Model for Metal

The Drude model is commonly used to describe the complex relative permittivity for metals. The complex relative permittivity of multiple poles Drude model is

Figure 5.24: Real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity for metal Au (gold): Drude-Lorentz model and experimental data.

expressed as

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{-\omega_{D,p}^2}{\omega^2 - j\omega\nu_p}. \quad (5.5.1)$$

In [167], the author first tried to fit the complex relative permittivity of metal Au (gold) with a single pole Drude model using the data tabulated from [168] for photon energy between 1.24 eV (wavelength 1000 nm) and 2.48 eV (500 nm). The relevant parameters of the Drude model is listed in the first row of Table 5.8. The real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity are plotted in Fig. 5.23, along with the tabulated data. We first note that the imaginary part is negative for losses and absorption in metal. The real part is also negative for most metals at frequency below the plasma frequency. It can be seen that the Drude model does not fit the complex permittivity data accurately above energy level of 2 eV (600 nm).

To overcome such inaccuracy, additional Lorentz pole pairs can be added to take into account the interband transitions. In fact, the complex relative permittivity of several types of metal at optical frequency can be described more accurately by a

Figure 5.25: Real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity for metal Ag (silver): Drude-Lorentz model and experimental data.

combination of Drude-Lorentz model [169]. A Drude-Lorentz model with multiple poles are expressed as

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_p \frac{-\omega_{D,p}^2}{\omega^2 - j\omega\nu_p} + \sum_p \frac{\Delta\epsilon_p\omega_{L,p}^2}{\omega_{L,p}^2 + 2j\omega\delta_p - \omega^2}. \quad (5.5.2)$$

The authors in [167] fitted the complex relative permittivity of metal Au (gold) with a combination of one Drude pole and one Lorentz pole pair for photon energy range between 1.24 eV and 2.48 eV. The relevant parameters of Drude-Lorentz model for metal Au are listed in the second row of Table 5.8. Fig. 5.24 now plots the real, ϵ_{rr} and imaginary, ϵ_{ri} parts of the complex relative permittivity for metal Au using Drude-Lorentz model, along with the same tabulated data in [168]. It can be seen now that the Drude-Lorentz model fits the data accurately beyond energy level of 2 eV, which validates the accuracy of the Drude-Lorentz model.

We next consider the complex relative permittivity of metal Ag (silver). [169] provided the fitting of complex relative permittivity for 11 types of metal, including Ag using a combination of single Drude pole and multiple Lorentz pole pairs for a wide photon energy range from 0.1 eV to 5 eV. The compilation of complex relative per-

Table 5.8: Parameters of Drude and Drude-Lorentz models for metal Au (gold)

Au	ϵ_∞	$\omega_{D,1}(\text{rad/s})$	$\nu_1(\text{rad/s})$	$\Delta\epsilon_1$	$\omega_{L,1}(\text{rad/s})$	$\delta_1(\text{rad/s})$
Drude	9.0685	1.3544×10^{16}	1.1536×10^{14}	-	-	-
Drude-Lorentz	5.9673	1.3280×10^{16}	1.0003×10^{14}	1.09	4.0845×10^{15}	3.2943×10^{14}

Table 5.9: Parameters of Drude-Lorentz model for metal Ag (silver)

Ag	ϵ_∞	$\omega_{D,1}(\text{rad/s})$	$\nu_1(\text{rad/s})$	$\Delta\epsilon_p(p=1,2)$	$\omega_{L,p}(p=1,2)(\text{rad/s})$	$\delta_p(p=1,2)(\text{rad/s})$
Drude-Lorentz	1	1.2583×10^{16}	7.2923×10^{13}	5.9245	1.2397×10^{15}	0.3519×10^{15}
	-	-	-	1.4013	6.8078×10^{15}	1.4334×10^{14}

mittivity data are obtained from [170]. For a shorter energy range between 1.24 eV and 2.48 eV, we manage to reduce the order of the Drude-Lorentz model from one Drude pole and five Lorentz pole pairs in [169] to one Drude pole and two Lorentz pole pairs. Such reduced order of Drude-Lorentz model is more desirable to be used in FADI-FDTD method for simplicity and efficiency. The relevant parameters of Drude-Lorentz model for metal Ag are listed in Table 5.9. Fig. 5.25 shows the the real, ϵ_{rr} and imaginary parts ϵ_{ri} of the complex relative permittivity for metal Ag using Drude-Lorentz model, along with the tabulated data in [170]. It can be seen that our reduced order of Drude-Lorentz model fits the data well within photon energy of 1.24 eV and 2.48 eV.

5.5.2 Numerical Results

For numerical demonstrations, we consider a 2-D optical waveguide with length of 10 μm and width of 0.4 μm where a core is confined between two metal claddings. The core is air (free space) having width of 0.2 μm and the two metal claddings are made of Au (gold) having Drude-Lorentz model parameters in Table 5.8. A transverse magnetic (TM) modulated Gaussian pulse with wavelengths 500 nm to 1000 nm (photon energy 1.24 eV to 2.48 eV) is excited in the core region and the pulse is allowed to propagate along the waveguide. Cell size Δ is chosen as 0.005 μm

Figure 5.26: Magnitude of transmission coefficient of the optical waveguide from photon energy 1.24 eV to 2.48 eV for various CFLNs.

Table 5.10: Efficiency gain and relative error of FADI-FDTD method for various CFLNs

CFLN	2	4	6	8	10
Efficiency gain	1.67	3.33	5.00	6.66	8.33
Relative error	0.29%	0.59%	1.18%	1.91%	2.86%

which corresponds to CPW of 100 at $5 \mu\text{m}$ and the time step Δt is specified as CFLN defined earlier. In this study, we compute the transmission coefficient of the optical waveguide by taking the ratio of Fourier transformed fields observed between two different points at the core centre separated by $5 \mu\text{m}$ along the waveguide length. The numerical experiment is run for various CFLNs to validate the accuracy FADI-FDTD method under different time steps.

Fig. 5.26 shows the magnitude of transmission coefficient of the optical waveguide from photon energy 1.24 eV to 2.48 eV for various CFLNs. Also shown in the figure is the transmission coefficient computed using the Yee's explicit FDTD method to serve as reference. Since the Yee's explicit FDTD method is not unconditionally stable, it is run at its maximum time step limit of CFLN=1. The results are quite agreeable

Table 5.11: Relative error of efficient FADI-FDTD schemes for various CFLNs and CPWs

CFLN		2	4	6	8	10
CPW	50	0.37%	1.71%	4.04%	7.51%	12.54%
	100	0.29%	0.59%	1.18%	1.91%	2.86%

and close to each other. As the CFLN increases, the magnitude of transmission coefficient computed using FADI-FDTD method deviates further away from the reference. To illustrate the trade-off between accuracy and efficiency, Table 5.10 shows the efficiency gain and relative error of FADI-FDTD method. The efficiency gain is taken over the Yee's explicit FDTD and the relative error is computed as

$$err = \left| \frac{T_{FADI} - T_{explicit}}{T_{explicit}} \right| \quad (5.5.3)$$

where T_{FADI} and $T_{explicit}$ are the magnitude of transmission coefficients computed using FADI-FDTD and Yee's explicit FDTD methods respectively. The transmission coefficient is computed at centre photon energy of 1.9 eV. It can be seen that at CFLN=10, the FADI-FDTD method is 8.33 times faster than the Yee's explicit FDTD method at the expense of only 2.35 percent relative error. Hereby, we compare the efficiency gain of our FADI-FDTD with that of LOD-FDTD method proposed in [171]. For the same numerical experiment at CFLN=7, the authors in [171] reported that the simulation time of LOD-FDTD is reduced to 39 percent of the Yee's explicit FDTD counterpart. For our FADI-FDTD method, with the same CFLN, the simulation time is further reduced to only 17.15 percent of Yee's explicit FDTD counterpart. Furthermore, the temporal accuracy of LOD-FDTD is only up to first-order while our FADI-FDTD has temporal accuracy of up to second-order. Table 5.11 further shows the relative error of FADI-FDTD method for various CFLNs under different CPWs. It can be seen that for the same CFLN but at a lower CPW of 50, the relative error increases.

Figure 5.27: Magnitude of transmission coefficient of the optical waveguide whereby its gold metal cladding is modeled separately as Drude-Lorentz and Drude model.

For comparison, Fig. 5.27 plots the the magnitude of transmission coefficient of the optical waveguide whereby its gold metal cladding is modeled separately as Drude-Lorentz and Drude model. The numerical experiment is conducted at CFLN=8. Significant difference of transmission coefficient magnitude can be seen above photon energy of 1.8 eV. This further indicates the inaccuracy of Drude model for gold. The Drude-Lorentz model should be employed for analysis of optical waveguide with gold as its metal cladding.

Previously we have considered Au-air-Au interface for the optical waveguide. We further investigate the transmission response of the optical waveguide using different metal and material types as its cladding and core. We first consider Ag-air-Ag interface, Fig. 5.28 plots the magnitude of transmission coefficients of optical waveguide with Ag-air-Ag interface and compares it with Au-air-Au interface. Ag (silver) is modeled as Drude-Lorentz model having parameters from Table 5.9. The numerical experiment is again conducted at CFLN=8. It can be seen that for Au-air-Au interface, no electromagnetic wave with photon energy above 2.4 eV can propagate beyond 5 μm of the optical waveguide, indicated by its zero transmission coefficient

Figure 5.28: Magnitude of transmission coefficients of the optical waveguide with Au-air-Au and Ag-air-Ag interfaces.

for photon energy above 2.4 eV. For Ag-air-Ag interface, the magnitude of transmission coefficient is relatively higher throughout the photon energy from 1.24 eV to 2.48 eV, which indicates that most electromagnetic wave can propagate through the optical waveguide. Finally, we replace the core in the optical waveguide with silicon dioxide (SiO_2) having constant refractive index of 1.444 [75]. Fig. 5.29 plots the magnitude of transmission coefficients of the optical waveguide with Au- SiO_2 -Au and Au-air-Au interfaces. We can see that for Au- SiO_2 -Au interface, the magnitude of transmission coefficient is reduced compared to that of Au-air-Au interface. No electromagnetic wave with photon energy above 2.2 eV can now propagate beyond $5 \mu\text{m}$ of the optical waveguide.

We next proceed to analyze plasmonic waveguide grating filter [172, 173], which is formed by periodic width variation of insulator as its core, and encapsulated by metal as its cladding. It is one of the basic building blocks for small size plasmonic circuit. Fig. 5.30 shows the configurations of conventional plasmonic waveguide grating filter [173]. The dimensions are: $W_1 = 0.1 \mu\text{m}$, $W_2 = 0.2 \mu\text{m}$, $L_p = 0.66 \mu\text{m}$, $L_s = 0.292 \mu\text{m}$. The number of periods is chosen as 19. We shall analyze such

Figure 5.29: Magnitude of transmission coefficients of the optical waveguide with Au-air-Au and Au-SiO₂-Au interfaces.

Figure 5.30: Configurations of conventional plasmonic waveguide grating filter. ©2010 IEEE.

plasmonic waveguide grating filter in the wavelength region of $1.2 \mu m$ to $2.4 \mu m$, which corresponds to photon energy of 0.52 eV to 1.1 eV . The metal is chosen as Ag in which a Drude model is sufficient for the aforementioned photon energy range, having parameters: $\epsilon_{\infty} = 3.7$, $\omega_{D,1} = 1.3825 \times 10^{16} \text{ rad/s}$ and $\nu_1 = 2.7347 \times 10^{13} \text{ rad/s}$. A TM modulated Gaussian pulse with the aforementioned photon energy range is excited in the core region and the pulse is allowed to propagate along the waveguide. Nonuniform cell size is chosen where $\Delta z = 0.004 \mu m$ and $\Delta x = 0.005 \mu m$.

Figure 5.31: Magnitude of transmission coefficient of conventional plasmonic waveguide grating filter from photon energy 0.52 eV to 1.1 eV.

CFLN is set at 4. Fig. 5.31 shows the transmission coefficient of the conventional plasmonic waveguide grating filter from photon energy of 0.52 eV to 1.1 eV. For comparison, we also present the results obtained by Yee's explicit FDTD method. It can be seen that both results agree with each other satisfactorily and the FADI-FDTD method is thus validated. From Fig. 5.31, it is observed that with such configuration, the bandgap energy starts around 0.65 eV and ends around 0.9 eV. Considerable high sidelobes and ripples can be seen at the passband region.

Figure 5.32: Configurations of apodized plasmonic waveguide grating filter. ©2010 IEEE.

Figure 5.33: Magnitude of transmission coefficient of apodized plasmonic waveguide grating filter from photon energy 0.52 eV to 1.1 eV.

Figure 5.34: Configurations of chirped plasmonic waveguide grating filter. ©2010 IEEE.

To suppress the sidelobes level, it is proposed in [173] that apodization be introduced into the plasmonic waveguide grating filter. Fig. 5.32 shows the configurations of the apodized plasmonic waveguide grating filter, where linear apodization is applied at both input and output ports. CFLN is chosen at 10 henceforth for greater efficiency. Fig. 5.33 now plots the transmission coefficients of the apodized filter with linear apodization applied to 5 and 9 periods at both input and output ports. With apodization, we can see that the sidelobes level are suppressed and reduced

Figure 5.35: Magnitude of transmission coefficient of chirped plasmonic waveguide grating filter from photon energy 0.52 eV to 1.1 eV.

where a smoother passband is depicted. Nevertheless, this comes at the expense of a narrower bandgap. Generally, higher number of periods will contribute to lower sidelobes level with narrower bandgap as can be seen from the comparison between apodized filter with 5 and 9 periods. Apart from apodization, the use of chirped grating can also achieve the same objective in suppressing the sidelobes level. The configuration of a typical linear chirped plasmonic waveguide grating filter is shown in Fig. 5.34. Fig. 5.35 plots the transmission coefficients of the chirped filter with linear chirped applied to 5 and 9 periods at both input and output ports. We can also see that the sidelobes level can be suppressed and reduced. Similarly, higher number of periods will contribute to lower sidelobes level with narrower bandgap.

Finally, we consider a plasmonic microcavity in which a defect section is introduced in the middle section of the waveguide, both conventional and apodized, as depicted in Fig. 5.36 and Fig. 5.37, respectively. The defect length is chosen as $L = 0.688\mu\text{m}$ and the number of gratings is 18. Fig. 5.38 now shows the transmission coefficient of the conventional plasmonic microcavity, as well as the apodized microcavity in 6 and 8 periods. When a defect is introduced in the middle section of the waveguide, a

Figure 5.36: Configurations of conventional plasmonic microcavity. ©2010 IEEE.

Figure 5.37: Configurations of apodized plasmonic microcavity. ©2010 IEEE.

transmission peak can be observed at its bandgap at around photon energy 0.78 eV. Sidelobes level suppression can also be achieved by apodization in the microcavity. As the number of period increases, the sidelobes level decreases at the expense of narrower bandgap. At the same time, the transmission peak at 0.78 eV increases as the apodization period increases.

Figure 5.38: Magnitude of transmission coefficient of apodized plasmonic microcavity from photon energy 0.52 eV to 1.1 eV.

5.6 Conclusions

The applications of FADI-FDTD method for lossy and dispersive media mainly in the areas of electromagnetic compatibility, bioelectromagnetics, as well as photonics have been demonstrated. In electromagnetic compatibility, the modeling of reverberation chamber in mode-stirred operation has been presented. A time variant complex relative permittivity has been introduced such that the boundary conditions inside the chamber can be altered continuously, i.e., the mode-stirred operation. For application in bioelectromagnetics, the interaction of light with hemoglobin at optical frequency has been presented. An accurate model based on complex conjugate pole-residue pairs has been proposed to model the complex permittivity of hemoglobin at optical frequency. Besides that, the interaction of terahertz pulse with healthy skin and BCC has been demonstrated, where the human skin is modeled as Debye media. For application in photonics, the characteristics of a surface plasmon waveguides with Au (gold) and Ag (silver) metal cladding, modeled as combination of Drude-Lorentz dispersive media have been analyzed. Further analysis of plasmonic waveguide grating filter has also been considered.

Chapter 6

Conclusions and Future Work

6.1 Conclusions

This thesis has presented the analysis and applications of FDTD methods for lossy and dispersive media. The stability analysis is first performed on explicit FDTD schemes for doubly lossy media whereby a generalized stability criterion applicable for all 3-D explicit FDTD schemes has been found. Similarly, the 3-D dispersion analysis has revealed some important dispersion characteristics of 3-D explicit FDTD schemes for doubly lossy media. The thesis has also proposed a corrected impulse invariance method as the current classical impulse invariance method used in explicit FDTD for dispersive media is found to be inaccurate. A corrected Z-transform table has been provided to facilitate the conversion from frequency to Z domain. With the aid of the table, various formulations of FDTD update equations for dispersive media can be carried out conveniently.

For unconditionally stable ADI-FDTD method, Lyapunov and matrix norm stability analysis has been applied on various ADI schemes for doubly lossy media. A rigorous analytical proof of unconditional stability has been provided. Subsequently, an unified efficient FADI-FDTD schemes for lossy media has been formulated. They have been formulated in the simplest, most concise, most efficient, and most funda-

mental form of ADI-FDTD. Such efficient fundamental schemes have substantially less RHS update coefficients and field variables compared to the conventional ADI-FDTD schemes. Thus, they feature higher efficiency with reduced memory indexing and arithmetic operations. The generalized formulation of FADI-FDTD method for dispersive media has also been provided. It is efficient, robust and applicable to Debye, Lorentz, Drude and general complex conjugate pole-residue pair models.

The applications FADI-FDTD method have been demonstrated in the areas of electromagnetic compatibility, bioelectromagnetics and photonics. In electromagnetic compatibility, the modeling of reverberation chamber in mode-stirred operation has been presented. A time variant complex relative permittivity has been introduced such that the boundary conditions inside the chamber can be altered continuously, i.e., the mode-stirred operation. For application in bioelectromagnetics, the interaction of light with hemoglobin at optical frequency has been presented. An accurate model based on complex conjugate pole-residue pairs has been proposed to model the complex permittivity of hemoglobin at optical frequency. The interaction of terahertz pulse with healthy skin and BCC has been demonstrated, where the human skin is modeled as Debye media. For application in photonics, the characteristics of an optical waveguide with Au (gold) and Ag (silver) metal cladding, modeled as combination of Drude-Lorentz dispersive media have been analyzed. Further analysis of plasmonic waveguide grating filter has also been considered.

The comparison among Yee's explicit FDTD, ADI-FDTD and FADI-FDTD methods are summarized in Table 6.1. Some of the compared features are implicit/explicit, stability, number of substep, complexity of right-hand-side (RHS), source excitation, etc. The main advantage of Yee's explicit FDTD method is the simplicity due to its explicit nature, which comes along with simple update equations, less flops count and memory indexing. Nevertheless, the Yee's explicit FDTD method is not uncon-

ditionally stable, the time step is restricted by the CFL condition, which imposes a constraint on it depending on the mesh size. For a fine mesh or nonuniform cell size, the time step is greatly hindered by the smaller cell size and this can result in undesirably long simulation time and hence reduces the computation efficiency. The ADI-FDTD method on the other hand is unconditionally stable, in which its time step is no longer restricted by the cell size. However, the complicated nature of the algorithm, often also results in low computation efficiency because of its implicit nature, and its flops count and memory indexing is far greater than that of the Yee's explicit FDTD method. The FADI-FDTD method has addressed the above dilemma by combining both advantages of simplicity and unconditional stability. It is implicit in nature but have a matrix-free-operator RHS, which results in reduced flops count, memory indexing, programming simplicity, etc. While maintaining unconditional stability, the FADI-FDTD still allows for efficient electromagnetic computation in dealing with lossy and dispersive media. As final conclusion, the thesis has successfully developed a comprehensive FDTD-based computational framework which serves as a modeling and analysis platform for lossy and dispersive electromagnetic problems.

Table 6.1: Comparison among Yee's explicit FDTD, ADI-FDTD and FADI-FDTD methods

	Yee's Explicit FDTD	ADI-FDTD	FADI-FDTD
Implicit/explicit	Explicit	Implicit	Implicit
Stability	Not unconditionally stable	Unconditionally stable	Unconditionally stable
Number of substep	One	Two	Two
Right-hand-side (RHS)	<ul style="list-style-type: none"> -Simple -Less flops count and memory indexing -Programming simplicity 	<ul style="list-style-type: none"> -Complicated -Not matrix-operator-free -More flops count and memory indexing -No programming simplicity 	<ul style="list-style-type: none"> -Simple -Matrix-operator-free -Most concise, most fundamental -Reduced flops count and memory indexing -Programming simplicity
Source excitation	Required only in one substep.	Required in two substeps	Required only in one substep
More specifically on lossy media	<ul style="list-style-type: none"> -Unified form -Generalized stability analysis for doubly lossy media using von Neumann eigenvalue approach -More relaxed stability criterion for TF and ETD schemes, more stringent stability criterion for TB scheme -Update coefficients of E field update equations does not involve magnetic conductivity, c.f. (2.2.2a)-(2.2.2c) 	<ul style="list-style-type: none"> -Unified in conventional form -Generalized stability analysis for doubly lossy media using Lyapunov and matrix norm approach -Unconditionally stable for all schemes except backward-backward scheme -Update coefficients of RHS E field implicit update equations involve magnetic conductivity, c.f. (2.3.6a)-(2.3.6c), (2.3.7a)-(2.3.7c) 	<ul style="list-style-type: none"> -Unified in fundamental form -Generalized stability analysis for doubly lossy media using Lyapunov and matrix norm approach -Unconditionally stable for all schemes except backward-backward scheme -Update coefficients of RHS E field implicit update equations does not involve magnetic conductivity, c.f. (4.7.5a)-(4.7.5c), (4.7.8a)-(4.7.8c)

	-Simple update equations	-Complicated update equations	-Simple update equations
More specifically on dispersive media	-Not in unified form -Dispersive terms J and M required separately in either explicit E or H field update equations, c.f. (2.2.29), (2.2.36), (2.2.44)	-Unified in conventional form -Dispersive terms J and M both required simultaneously in E field implicit update equations, c.f. (4.9.14)	-Unified in fundamental form -Dispersive terms J and M only required separately in auxiliary update equations. No J and M required in E field implicit update equations, c.f. (4.9.41).
	-Simple update equations	-Complicated update equations	-Simple update equations

6.2 Suggestions for Future Work

Although extensive studies have been conducted on FDTD methods for lossy and dispersive media, there are still other interesting areas which can be further explored. Some suggestions for future work are as follows.

Preliminary studies have shown that the matrix exponential method exhibits promising high accuracy in explicit FDTD method for Debye media [174]. Therefore, the matrix exponential method can be extended and further incorporated into our generalized FADI-FDTD method for dispersive media based on the generalized formulation in Chapter 4. On top of that, some biological tissues are more suitably characterized by the Cole-cole model [175] and its incorporation into our FADI-FDTD method is highly desired.

The analytical proof of unconditional stability of ADI-FDTD method for dispersive media remains elusive. However, based on the foundation and framework on Lyapunov and matrix norm stability laid out in Chapter 4, they can be further

extended into stability analysis of ADI-FDTD method for the most general case of doubly dispersive media.

Our FADI-FDTD method offers wide opportunity for further extensions and combinations with other time domain based methods. For instance, the pseudospectral time domain (PSTD) method [176], which offers high accuracy in terms of spatial sampling can be further extended into our FADI-FDTD method. Besides, incorporation can also be done for the unconditionally stable complex envelope (CE) ADI-FDTD method [177], which is suitable for high frequency but narrowband problems. The formulation of focused beam propagation [178] in our FADI-FDTD method can also be attempted for more detail studies of interaction of electromagnetic wave with biological matter at cellular level.

Recently, the graphic processing unit (GPU) has been exploited to further boost the computational efficiency of FDTD methods [179]. It is therefore of great interest to explore the usability of GPU in our FADI-FDTD method. With such highly efficient FADI-FDTD method, other increasingly popular topics of photonic crystal structures [180] and metamaterials [181] can also be ventured into. In short, the prominent features of our FADI-FDTD method will greatly facilitate the research in other useful engineering and science applications.

Author's Publications

Journal Papers

1. D. Y. Heh and E. L. Tan, "Modeling the interaction of terahertz pulse with healthy skin and basal cell carcinoma using the unconditionally stable fundamental ADI-FDTD method," *Progress In Electromagnetics Research B*, vol. 37, pp. 365–386, 2012.
2. D. Y. Heh and E. L. Tan, "Unified efficient fundamental ADI-FDTD schemes for lossy media," *Progress In Electromagnetics Research B*, vol. 32, pp. 217–242, 2011.
3. D. Y. Heh and E. L. Tan, "Modeling hemoglobin at optical frequency using the unconditionally stable fundamental ADI-FDTD method," *Biomed. Opt. Express*, vol. 2, no. 5, pp. 1169–1183, May 2011.
4. D. Y. Heh and E. L. Tan, "Lyapunov and matrix norm stability analysis of ADI-FDTD schemes for doubly lossy media," *IEEE Trans. Antennas Propagat.*, vol. 59, no. 3, pp. 979–986, Mar. 2011.
5. W. C. Tay, D. Y. Heh and E. L. Tan, "GPU-accelerated fundamental ADI-FDTD with complex frequency shifted convolutional perfectly matched layer," *Progress In Electromagnetics Research M*, vol. 14, pp. 177–192, 2010.
6. D. Y. Heh and E. L. Tan, "Generalized stability criterion of 3-D FDTD schemes for doubly lossy media," *IEEE Trans. Antennas Propagat.*, vol. 58, no. 4, pp. 1421–1425, Apr. 2010.
7. D. Y. Heh and E. L. Tan, "Corrected impulse invariance method in Z-transform theory for frequency-dependent FDTD methods," *IEEE Trans. Antennas Propagat.*, vol. 57, no. 9, pp. 2683–2690, Sep. 2009. **(First runner up for IEEE Singapore MTT/AP Chapter Best Student Paper Award)**

8. D. Y. Heh and E. L. Tan, "Dispersion analysis of FDTD schemes for doubly lossy media," *Progress In Electromagnetics Research B*, vol. 17, pp. 327–342, 2009.
9. D. Y. Heh and E. L. Tan, "FDTD modeling for dispersive media using matrix exponential method," *IEEE Microw. Wireless Compon. Lett.*, vol. 19, no. 2, pp. 53–55, Feb. 2009.
10. E. L. Tan and D. Y. Heh, "ADI-FDTD method with fourth order accuracy in time," *IEEE Microw. Wireless Compon. Lett.*, vol. 18, no. 5, pp. 296–298, May 2008.

Conference Papers

1. D. Y. Heh and E. L. Tan, "Efficient implementation of 3-D ADI-FDTD method for lossy media," *IEEE MTT-S Intl. Microw. Symp. Digest*, pp. 313–316, 2009.
2. D. Y. Heh and E. L. Tan, "Modeling debye dispersive media using efficient ADI-FDTD method," *IEEE AP-S Intl. Symp. Digest*, art. no. 5172058, 2009.
3. D. Y. Heh and E. L. Tan, "Modeling lorentz dispersive media in FDTD using the exponential time differencing method," *Proc. of 2008 Asia Pacific Microw. Conf.*, art. no. 4958061, 2008. **(Shortlisted for Best Student Paper Award)**
4. D. Y. Heh and E. L. Tan, "Split-Step Finite-Difference Time-Domain method with fourth order accuracy in time," *2008 Asia-Pacific Symp. on Electromag. Compat. and 19th Intl. Zurich Symp. on Electromag.Compat.*, pp. 68–71, 2008.
5. E. L. Tan and D. Y. Heh, "Corrected impulse invariance method for dispersive media using FDTD," *2008 Asia-Pacific Symp. on Electromag. Compat. and 19th Intl. Zurich Symp. on Electromag.Compat.*, pp. 56–59, 2008.

Bibliography

- [1] K. S. Yee, "Numerical solution of initial boundary value problems involving Maxwell's equation in isotropic media," *IEEE Trans. Antennas Propagat.*, vol. 14, no. 4, pp. 302–307, Apr. 1966.
- [2] A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method* Boston, M. A.: Artech House, 2005.
- [3] F. Zheng, Z. Chen, and J. Zhang, "Toward the development of a three-dimensional unconditionally stable finite-difference time-domain method," *IEEE Trans. Microw. Theory Tech.*, vol. 48, no. 9, pp. 1550–1558, Sep. 2000.
- [4] T. Namiki, "3-D ADI-FDTD method: unconditionally stable time-domain algorithm for solving full vector maxwell's equations," *IEEE Trans. Microw. Theory Tech.*, vol. 48, no. 9, pp. 1743–1748, Oct. 2000.
- [5] R. Luebbers, K. Kumagai, S. Adachi and T. Uno, "FDTD calculation of transient pulse propagation through a nonlinear magnetic sheet," *IEEE Trans. Electromagn. Compat.*, vol. 35, no. 1, pp. 90–94, Feb. 1993.
- [6] A. Taflove and M. E. Brodwin, "Numerical solution of steady-state electromagnetic scattering problems using the time-dependent Maxwell's equations," *IEEE Trans. Microw. Theory Tech.*, vol. 23, no. 8, pp. 623–630, Aug. 1975.
- [7] R. Holland, L. Simpson and K. S. Kunz, "Finite-difference analysis of EMP coupling to lossy dielectric structures," *IEEE Trans. Electromagn. Compat.*, vol. 22, no. 3, pp. 203–209, Aug. 1980.
- [8] P. G. Petropoulos, "Analysis of exponential time-differencing for FDTD in lossy dielectrics," *IEEE Trans. Antennas Propagat.*, vol. 45, no. 6, pp. 1054–1057, Jun. 1997.
- [9] C. L. Wagner and J. B. Schneider, "Divergent fields, charge, and capacitance in FDTD simulations," *IEEE Trans. Microw. Theory Tech.*, vol. 46, no. 12, pp. 2131–2136, Dec. 1998.
- [10] S. C. Winton, P. Kosmas and C. M. Rappaport, "FDTD simulation of TE and TM plane waves at nonzero incidence in arbitrary layered media," *IEEE Trans. Antennas Propagat.*, vol. 53, no. 5, pp. 1721–1728, May 2005.
- [11] P. Kosmas, "Review of an FDTD TF/SF formulation based on auxiliary 1-D grids," *2007 Workshop on Computational Electromagnetics in Time-Domain, CEM-TD.*, art. no. 4373540 2007.

- [12] Y. N. Jiang, D. B. Ge and S. J. Ding, "Analysis of TF-SF boundary for 2D-FDTD with plane p-wave propagation in layered dispersive and lossy media," *Progress In Electromagnetics Research B*, vol. 83, pp. 157–172, 2008.
- [13] J. P. Berenger, "A perfectly matched layer for the absorption of electromagnetic waves," *J. Computational Phys.*, vol. 114, pp. 185–200, 1994.
- [14] D. S. Katz, E. T. Thiele and A. Taflove, "Validation and extension to three dimensions of Berenger PML absorbing boundary condition for FD-TD meshes," *IEEE Microw. Guided Wave Lett.*, vol. 4, no. 8, pp. 268–270, Aug. 1994.
- [15] J. D. Moerlose and M. A. Stuchly, "Behavior of Berenger's ABC for evanescent waves," *IEEE Microw. Guided Wave Lett.*, vol. 5, no. 10, pp. 344–346, Oct. 1995.
- [16] J. Fang and Z. Wu, "Generalized perfectly matched layer-an extension of Berenger's perfectly matched layer boundary condition," *IEEE Microw. Guided Wave Lett.*, vol. 5, no. 12, pp. 451–453, Dec. 1995.
- [17] D. M. Sullivan, "A simplified PML for use with the FDTD method," *IEEE Microw. Guided Wave Lett.*, vol. 6, no. 2, pp. 97–99, Feb. 1996.
- [18] J. Fang and Z. Wu, "Generalized perfectly matched layer for the absorption of propagating and evanescent waves in lossless and lossy media," *IEEE Trans. Microw. Theory Tech.*, vol. 44, no. 12, pp. 2216–2222, Dec. 1996.
- [19] D. M. Sullivan, "An unsplit step 3-D PML for use with the FDTD method," *IEEE Microw. Guided Wave Lett.*, vol. 7, no. 7, pp. 184–186, Jul. 1997.
- [20] T. Uno, Y. He and S. Adachi, "Perfectly matched layer absorbing boundary condition for dispersive medium," *IEEE Microw. Guided Wave Lett.*, vol. 7, no. 9, pp. 264–266, Sep. 1997.
- [21] F. L. Teixeira and W. C. Chew, "A general approach to extend Berenger's absorbing boundary condition to anisotropic and dispersive media," *IEEE Trans. Antennas Propagat.*, vol. 46, no. 9, pp. 1386–1387, Sep. 1998.
- [22] A. P. Zhao, "Generalized-material-independent PML absorbers used for the FDTD simulation of electromagnetic waves in 3-D arbitrary anisotropic dielectric and magnetic media," *IEEE Trans. Microw. Theory Tech.*, vol. 46, no. 10, pp. 1511–1513, Oct. 1998.
- [23] G. X. Fan and Q. H. Liu, "An FDTD algorithm with perfectly matched layers for general dispersive media," *IEEE Trans. Antennas Propagat.*, vol. 48, no. 5, pp. 637–646, May 2000.
- [24] J. A. Roden and S. D. Gedney, "Convolution PML (CPML): an efficient FDTD implementation of the CFS-PML for arbitrary media," *Microw. Opt. Technol. Lett.*, vol. 27, no. 5, pp. 334–339, Dec. 2000.
- [25] R. Luebbers, F. P. Hunsberger, K. S. Kunz, R. B. Standler and M. Schneider, "A frequency-dependent finite-difference time-domain formulation for dispersive materials," *IEEE Trans. Electromagn. Compat.*, vol. 32, no. 3, pp. 222–227, Aug. 1990.
- [26] R. Luebbers and F. Hunsberger, "FDTD for nth-order dispersive media," *IEEE Trans. Antennas Propagat.*, vol. 40, no. 11, pp. 1297–1301, Nov. 1992.

- [27] D. F. Kelley and R. Luebbers, "Piecewise linear recursive convolution for dispersive media using FDTD," *IEEE Trans. Antennas Propagat.*, vol. 44, no. 6, pp. 791–797, Jun. 1996.
- [28] R. Siushansian and J. LoVetri, "A comparison of numerical techniques for modeling electromagnetic dispersive media," *IEEE Microw. Guided Wave Lett.*, vol. 5, no. 12, pp. 426–428, Dec. 1995.
- [29] Q. Chen, M. Katsurai and P.H. Aoyagi, "An FDTD formulation for dispersive media using a current density," *IEEE Trans. Antennas Propagat.*, vol. 46, no. 10, pp. 1739–1746, Oct. 1998.
- [30] S. Liu, N. Yuan and J. Mo, "A novel FDTD formulation for dispersive media," *IEEE Microw. Wireless Compon. Lett.*, vol. 13, no. 5, pp. 187–189, May 2003.
- [31] O. P. Gandhi, B. Gao and J. Chen, "A frequency-dependent finite-difference time-domain formulation for general dispersive media," *IEEE Trans. Microw. Theory Tech.*, vol. 41, no. 4, pp. 658–664, Apr. 1993.
- [32] J. L. Young, "Propagation in linear dispersive media: finite-difference time-domain methodologies," *IEEE Trans. Antennas Propagat.*, vol. 43, no. 4, pp. 422–426, Apr. 1995.
- [33] T. Kashiwa and I. Fukai, "A treatment by the FD-TD method of the dispersive characteristics associated with electronic polarization," *Microw. Opt. Technol. Lett.*, vol. 3, pp. 203–205, 1990.
- [34] R. M. Joseph, S. C. Hagness and A. Taflove, "Direct time integration of maxwell's equations in linear dispersive media with absorption for scattering and propagation of femtosecond electromagnetic pulses," *Opt. Lett.*, vol. 16, no. 18, pp. 1412–1414, Sep. 1991.
- [35] M. Okoniewski, M. Mrozowski and M.A. Stuchly, "Simple treatment of multi-term dispersion in FDTD," *IEEE Microw. Guided Wave Lett.*, vol. 7, no. 5, pp. 121–123, May 1997.
- [36] Y. Takayama and W. Klaus, "Reinterpretation of the auxiliary differential equation method for FDTD," *IEEE Microw. Wireless Compon. Lett.*, vol. 12, no. 3, pp. 102–104, Mar. 2002.
- [37] D. M. Sullivan, "Frequency-dependent FDTD methods using z transforms," *IEEE Trans. Antennas Propagat.*, vol. 40, no. 10, pp. 1223–1230, Oct. 1992.
- [38] D. M. Sullivan, "Z-transform theory and the FDTD method," *IEEE Trans. Antennas Propagat.*, vol. 44, no. 11, pp. 28–34, Jan. 1996.
- [39] W. H. Weedon and C. M. Rappaport, "A general method for FDTD modeling of wave propagation in arbitrary frequency-dispersive media," *IEEE Trans. Antennas Propagat.*, vol. 45, no. 3, pp. 401–410, Mar. 1997.
- [40] C. Rappaport, S. Wu, and S. Winton, "FDTD wave propagation in dispersive soil using a single pole conductivity model," *IEEE Trans. Magn.*, vol. 35, no. 3, pp. 1542–1545, May 1999.
- [41] P. Kosmas and C. Rappaport, "Modeling with the FDTD method for microwave breast cancer detection," *IEEE Trans. Microw. Theory Tech.*, vol. 52, no. 8, pp. 1890–1897, Aug. 2004.

- [42] J. A. Pereda, A. Vegas and A. Prieto, "FDTD modeling of wave propagation in dispersive media by using the mobius transformation technique," *IEEE Trans. Microw. Theory Tech.*, vol. 50, no. 7, pp. 1689–1695, Jul. 2002.
- [43] K. P. Prokopidis, E. P. Kosmidou and T. D. Tsiboukis, "An FDTD algorithm for wave propagation in dispersive media using higher-order schemes," *J. Electromag. Waves Appl.*, vol. 18, no. 9, pp. 1171–1194, 2004
- [44] S. W. Samn, "Modeling dispersive dielectric media in FDTD: a systematic approach," *IEEE Trans. Antennas Propagat.*, vol. 53, no. 10, pp. 3367–3373, Oct. 2005.
- [45] J. L. Young and R. O. Nelson, "A summary and systematic analysis of FDTD algorithms for linearly dispersive media," *IEEE Antennas Propagat. Magazine*, vol. 43, no. 1, pp. 61–77, Feb. 2001.
- [46] F. L. Teixeira, "Time-domain finite-difference and finite-element methods for Maxwell equations in complex media," *IEEE Trans. Antennas Propagat.*, vol. 56, no. 8, pp. 2150–2166, Aug. 2008.
- [47] C. C.-P. Chen, T.-W. Lee, N. Murugesan and S. C. Hagness, "Generalized FDTD-ADI: An unconditionally stable full-wave maxwell's equations solver for VLSI interconnect modeling," *IEEE/ACM Int. Conf. on Computer Aided Design*, San Jose, CA, USA, Nov. 2000, pp. 156–163.
- [48] S. G. Garcia, T. W. Lee and S. C. Hagness, "On the accuracy of the ADI-FDTD method," *IEEE Antennas Wireless Propagat. Lett.*, vol. 1, no. 1, pp. 31–34, 2002.
- [49] W. Fu and E. L. Tan, "Stability and dispersion analysis for ADI-FDTD method in lossy media," *IEEE Trans. Antennas Propagat.*, vol. 55, no. 4, pp. 1095–1102, Apr. 2007.
- [50] Yuan, C. and Z. Chen, "Towards accurate time-domain simulation of highly conductive materials," *2002 IEEE MTT-S Int. Microwave Symp. Dig.*, Seattle, WA, USA, June 2002, pp. 1135–1138.
- [51] J. A. Pereda, A. Grande, O. Gonzalez and A. Vegas, "The 1D ADI-FDTD method in lossy media," *IEEE Antennas Wireless Propagat. Lett.*, vol. 7, pp. 477–480, 2008.
- [52] J. A. Pereda, A. Grande, O. Gonzalez and A. Vegas, "Analysis of two alternative ADI-FDTD formulations for transverse-electric waves in lossy materials," *IEEE Trans. Antennas Propagat.*, vol. 57, no. 7, pp. 2047–2054, Jul. 2009.
- [53] D. Y. Heh and E. L. Tan, "Efficient implementation of 3-D ADI-FDTD method for lossy media," *2009 IEEE MTT-S Int. Microwave Symp. Dig.*, Boston, Massachusetts, USA, June 2009, pp. 313–316.
- [54] J. Shibayama, M. Muraki, J. Yamauchi and H. Nakano, "Efficient implicit FDTD algorithm based on locally one-dimensional scheme," *Electron. Lett.*, vol. 41, no. 19, pp. 1046–1047, Sep. 2005.
- [55] E. L. Tan, "Unconditionally stable LOD-FDTD method for 3-D Maxwell's equations," *IEEE Microw. Wireless Compon. Lett.*, vol. 17, no. 2, pp. 85–87, Feb. 2007.

- [56] G. Sun and C. W. Trueman, "Unconditionally stable Crank-Nicolson scheme for solving two-dimensional Maxwell's equations," *Electron. Lett.*, vol. 39, no. 7, pp. 595–597, Apr. 2003.
- [57] G. Sun and C. W. Trueman, "Unconditionally-stable FDTD method based on Crank-Nicolson scheme for solving three-dimensional Maxwell equations," *Electron. Lett.*, vol. 40, no. 10, pp. 589–590, May 2004.
- [58] G. Sun and C. W. Trueman, "Efficient implementations of the Crank-Nicolson scheme for the finite-difference time-domain method," *IEEE Trans. Microw. Theory Tech.*, vol. 54, no. 5, pp. 2275–2284, May 2006.
- [59] E. L. Tan, "Efficient algorithms for Crank-Nicolson-based finite-difference time-domain methods," *IEEE Trans. Microw. Theory Tech.*, vol. 56, no. 2, pp. 408–413, Feb. 2008.
- [60] T. -W. Lee and S. C. Hagness, "Wave source conditions for the unconditionally stable ADI-FDTD method," *IEEE Antennas and Propagation Soc., AP-S Intl. Symp.*, vol. 4, 2001. pp. 142–145.
- [61] A. P. Zhao, "Two special notes on the implementation of the unconditionally stable ADI-FDTD method," *Microw. Opt. Technol. Lett.*, vol. 33, no. 4, pp. 273–277, May 2002.
- [62] S. G. Garcia, A. R. Bretones, R. G. Martin and S. C. Hagness, "Accurate implementation of current sources in the ADI-FDTD scheme," *IEEE Antennas Wireless Propagat. Lett.*, vol. 3, pp. 141–144, 2004.
- [63] S. Wang, "On the current source implementation for the ADI-FDTD method," *IEEE Microw. Wireless Compon. Lett.*, vol. 14, no. 11, pp. 513–515, Nov. 2004.
- [64] B. Donderici and F. L. Teixeira, "Symmetric source implementation for the ADI-FDTD method," *IEEE Trans. Antennas Propagat.*, vol. 53, no. 4, pp. 1562–1565, Apr. 2005.
- [65] E. L. Tan, "Concise current source implementation for efficient 3-D ADI-FDTD method," *IEEE Microw. Wireless Compon. Lett.*, vol. 17, no. 11, pp. 748–750, Nov. 2007.
- [66] K. S. Zheng and D. B. Ge, "Implementation of the total-field/scattered-field technique in the 2D ADI-FDTD," *J. Xidian University*, vol. 33, no. 2, pp. 205–211, Apr. 2006.
- [67] G. Liu and S. D. Gedney, "Perfectly matched layer media for an unconditionally stable three-dimensional ADI-FDTD method," *IEEE Microw. Guided Wave Lett.*, vol. 10, no. 7, pp. 261–263, Jul. 2000.
- [68] S. D. Gedney, G. Liu, J. A. Roden and A. Zhu, "Perfectly matched layer media with CFS for an unconditionally stable ADI-FDTD method," *IEEE Trans. Antennas Propagat.*, vol. 49, no. 11, pp. 1554–1559, Nov. 2001.
- [69] S. Wang and F. L. Teixeira, "An efficient PML implementation for the ADI-FDTD method," *IEEE Microw. Wireless Compon. Lett.*, vol. 13, no. 2, pp. 72–74, Feb. 2003.

- [70] R. G. Rubio, S. G. Garcia, A. R. Bretones and R. G. Martin, "Crank-Nicolson reformulation of ADI-FDTD PML extensions," *IEEE Antennas Wireless Propagat. Lett.*, vol. 5, pp. 357–360, 2006.
- [71] S. Gonzalez, R. G. Rubio, A. R. Bretones and R. G. Martin, "Extension of the ADI-FDTD method to debye media," *IEEE Trans. Antennas Propagat.*, vol. 51, no. 11, pp. 3183–3186, Nov. 2003.
- [72] X. T. Dong, N. V. Venkatarayalu, B. Guo, W. Y. Yin and Y. B. Gan, "General formulation of unconditionally stable ADI-FDTD method in linear dispersive media," *IEEE Trans. Microw. Theory Tech.*, vol. 52, no. 1, pp. 170–174, Jan. 2004.
- [73] L. Xu and N. Yuan, "PLJERC-ADI-FDTD method for isotropic plasma," *IEEE Microw. Wireless Compon. Lett.*, vol. 15, no. 4, pp. 277–279, Apr. 2005.
- [74] H. -X. Zheng "ADI-FDTD formulation for general dispersive media," *IEEE Antennas and Propagation Soc., AP-S Intl. Symp.* art. no. 1710896, pp. 1723–1726, 2006.
- [75] K. -Y. Jung and F. L. Teixeira, "Multispecies ADI-FDTD algorithm for nanoscale three-dimensional photonic metallic structures," *IEEE Photonics Tech. Lett.*, vol. 19, no. 8, pp. 586–588, Apr. 2007.
- [76] J. A. Pereda, O. Gonzalez, A. Grande and A. Vegas, "An alternating-direction implicit FDTD modeling of dispersive media without constitutive relation splitting," *IEEE Microw. Wireless Compon. Lett.*, vol. 18, no. 11, pp. 719–721, Nov. 2008.
- [77] J. D. Hoffman, *Numerical methods for engineers and scientists* McGraw-Hill, 1993.
- [78] J. A. Pereda, O. Garcia, A. Vegas and A. Prieto, "Numerical dispersion and stability analysis of the FDTD technique in lossy dielectrics," *IEEE Microw. Guided Wave Lett.*, vol. 8, no. 7, pp. 245–247, Jul. 1998.
- [79] L. F. Velarde, J. A. Pereda, A. Vegas and O. Gonzalez, "A weighted-average scheme for accurate FDTD modeling of electromagnetic wave propagation in conductive media," *IEEE Antennas Wireless Propagat. Lett.*, vol. 3, pp. 302–305, 2004.
- [80] C. Schuster, A. Christ and W. Fichtner, "Review of FDTD time-stepping schemes for efficient simulation of electric conductive media," *Microw. Opt. Technol. Lett.*, vol. 25, no. 1, pp. 16–21, Apr. 2000.
- [81] P. G. Petropoulos, "Stability and phase error analysis of FD-TD in dispersive dielectrics," *IEEE Trans. Antennas Propagat.*, vol. 42, no. 1, pp. 62–69, Jan. 1994.
- [82] W. A. Beck and M. S. Mirotznik, "Generalized analysis of stability and numerical dispersion in the discrete-convolution FDTD method," *IEEE Trans. Antennas Propagat.*, vol. 48, no. 6, pp. 887–894, Jun. 2000.
- [83] J. A. Pereda, L. A. Vielva, A. Vegas and A. Prieto, "Analyzing the stability of the FDTD technique by combining the von Neumann method with the Routh-Hurwitz criterion," *IEEE Trans. Microw. Theory Tech.*, vol. 49, no. 2, pp. 377–381, Feb. 2001.

- [84] Z. Lin and L. Thylen, "On the accuracy and stability of several widely used FDTD approaches for modeling Lorentz dielectrics," *IEEE Trans. Antennas Propagat.*, vol. 57, no. 10, pp. 3378–3381, Oct. 2009.
- [85] B. Gustafsson, H. -O. Kreiss and J. Oliger *Time dependent problems and difference methods* New York: Wiley-Interscience, 1995.
- [86] B. Fornberg, "A short proof of the unconditional stability of the ADI-FDTD scheme," Univ. Colorado, Dept. Applied Mathematics, 2001, Technical Rep. 472.
- [87] S. Ogurtsov, G. Pan and R. Diaz, "Examination, clarification, and simplification of stability and dispersion analysis for ADI-FDTD and CNSS-FDTD schemes," *IEEE Trans. Antennas Propagat.*, vol. 55, no. 12, pp. 3395–3602, Dec. 2007.
- [88] S. G. Garcia, R. G. Rubio, A. Rubio Bretones and R. G. Lopez, "Revisiting the stability of Crank-Nicolson and ADI-FDTD," *IEEE Trans. Antennas Propagat.*, vol. 55, no. 11, pp. 3199–3203, Nov. 2007.
- [89] P. G. Petropoulos, "Phase error control for FD-TD methods of second and fourth order accuracy," *IEEE Trans. Antennas Propagat.*, vol. 42, no. 6, pp. 859–862, Jun. 1994.
- [90] J. L. Young, A. Kittichartphayak, Y. M. Kwok and D. Sullivan, "On the dispersion errors related to (FD)2TD type schemes," *IEEE Trans. Microw. Theory Tech.*, vol. 43, no. 8, pp. 1902–1910, Aug. 1995.
- [91] D. F. Kelley and R. J. Luebbers, "Calculation of dispersion errors for the piecewise linear recursive convolution method," *IEEE Antennas and Propagation Soc., AP-S Intl. Symp.*, vol. 3, pp. 1652–1655, 1996.
- [92] J. B. Schneider and C. L. Wagner, "FDTD dispersion revisited: faster-than-light propagation," *IEEE Microw. Guided Wave Lett.*, vol. 9, no. 2, pp. 54–56, Feb. 1999.
- [93] G. Sun and C. W. Trueman, "Numerical dispersion and numerical loss in explicit finite-difference time-domain methods in lossy media," *IEEE Trans. Antennas Propagat.*, vol. 53, no. 11, pp. 3684–3690, Nov. 2005.
- [94] T. Namiki and K. Ito, "Investigation of numerical errors of the two-dimensional ADI-FDTD method," *IEEE Trans. Microw. Theory Tech.*, vol. 48, no. 11, pp. 1950–1956, Nov. 2000.
- [95] F. Zheng and Z. Chen, "Numerical dispersion analysis of the unconditionally stable 3-D ADI-FDTD method," *IEEE Trans. Microw. Theory Tech.*, vol. 49, no. 5, pp. 1006–1009, May 2001.
- [96] A. P. Zhao, "Analysis of the numerical dispersion of the 2-D alternating-direction implicit FDTD method," *IEEE Trans. Microw. Theory Tech.*, vol. 50, no. 4, pp. 1156–1164, Apr. 2002.
- [97] M. Darms, R. Schuhmann, H. Spachmann and T. Weiland, "Dispersion and asymmetry effects of ADI-FDTD," *IEEE Microw. Wireless Compon. Lett.*, vol. 12, no. 12, pp. 491–493, Dec. 2002.

- [98] S. Ju, H. Kim and H. -H. Kim, "A study of the numerical dispersion relation for the 2-D ADI-FDTD method," *IEEE Microw. Wireless Compon. Lett.*, vol. 13, no. 9, pp. 405–407, Sep. 2003.
- [99] S. G. Garcia, R. G. Rubio, A. R. Bretones and R. G. Martin, "On the dispersion relation of ADI-FDTD," *IEEE Microw. Wireless Compon. Lett.*, vol. 16, no. 6, pp. 354–356, Jun. 2006.
- [100] S. G. Garcia, T. Lee and S. C. Hagness, "On the accuracy of the ADI-FDTD method," *IEEE Antennas Wireless Propagat. Lett.*, vol. 1, pp. 31–34, 2002.
- [101] M. K. Sun and W. Y. Tam, "Analysis of the numerical dispersion of the 2-D ADI-FDTD method with higher order scheme," *IEEE Antennas and Propagation Soc., AP-S Intl. Symp.*, vol. 4, pp. 348–351, 2003.
- [102] Z. Wang and J. Chen, "Analytical and numerical accuracy analysis of ADI-FDTD methods," *IEEE Antennas and Propagation Soc., AP-S Intl. Symp.*, vol. 4, pp. 344–347, 2003.
- [103] A. P. Zhao, "Consistency of the numerical dispersion relation expressed in different forms for the ADI-FDTD method," *Microw. Opt. Technol. Lett.*, vol. 40, no. 1, pp. 12–13, Jan. 2004.
- [104] V. Yurshevich and S. Lomov, "Measurement of magnetic spectra of ferrites: introducing a correction for ferrites dielectric parameters," *Measurement Science Review*, vol. 3, no. 3, pp. 41–44, 2003.
- [105] A. K. Singh, A. Verma, O. P. Thakur, C. Prakash, T. C. Goel and R. G. Mendiratta, "Electrical and magnetic properties of Mn-Ni-Zn ferrites processed by citrate precursor method," *Materials Lett.*, vol. 57, no. 5-6, pp. 1040–1044, Jan. 2003.
- [106] M. W. Hyde IV and M. J. Havrilla, "A nondestructive technique for determining complex permittivity and permeability of magnetic sheet materials using two flanged rectangular waveguides," *Progress In Electromagnetics Research*, vol. 79, pp. 367–386, 2008.
- [107] J. P. Y. Lee and K. G. Balmain, "Wire antennas coated with magnetically and electrically lossy material," *Radio Science*, vol. 14, no. 3, pp. 437–445, May 1979.
- [108] J.-H. Du, C. Sun, S. Bai, G. Su, Z. Ying, and H.-M. Cheng, "Microwave electromagnetic characteristics of a microcoiled carbon fibers/paraffin wax composite in Ku band," *Journal of Materials Research*, vol. 17, no. 5, pp. 1232–1236, May 2002.
- [109] F. Ulaby, *Fundamentals of Applied Electromagnetics, 5th Edition* Prentice Hall, 2007.
- [110] E. L. Tan and D. Y. Heh, "ADI-FDTD method with fourth order accuracy in time," *IEEE Microw. Wireless Compon. Lett.*, vol. 18, no. 5, pp. 296–298, May 2008.
- [111] L. B. Jackson, "A correction to impulse invariance," *IEEE Signal Processing Lett.*, vol. 7, no. 10, pp. 273–275, Oct. 2000.

- [112] W. F. G. Mecklenbrauker, "Remarks on and correction to the impulse invariant method for the design of IIR digital filters," *Signal Process.*, vol. 80, no. 10, pp. 1687–1690, Aug. 2000.
- [113] E. L. Tan and D. Y. Heh, "Corrected impulse invariance method for dispersive media using FDTD," *Proc. Asia-Pacific Symp. Electromagn. Compat.*, pp. 56–59, 2008.
- [114] William D. Hurt, "Multiterm debye dispersion relations for permittivity of muscle," *IEEE Trans. Biomed. Eng.*, vol. 42, no. 1, pp. 60–63, Jan. 1985.
- [115] W. Hahn, *Theory And Application Of Liapunov's Direct Method*. Englewood Cliffs, N. J.: Prentice-Hall, 1963.
- [116] A. Bacciotti and R. Lionel, *Liapunov Functions And Stability In Control Theory*, 2nd ed., Berlin, N. Y.: Springer, 2005.
- [117] P. J. Antsaklis and A. N. Michel, *Linear Systems*, New York: McGraw-Hill, 1997.
- [118] F. Ayres Jr., *Schaum's Outline Series Of Theory and Problems Of Matrices*. London, U. K.: McGraw-Hill, 1962.
- [119] G. D. Smith, *Numerical Solution Of Partial Differential Equations: Finite Difference Methods*, 3rd ed., Oxford, U. K.: Clarendon, 1985.
- [120] E. L. Tan, "Efficient algorithm for the unconditionally stable 3-D ADI-FDTD method," *IEEE Microw. Wireless Compon. Lett.*, vol. 17, no. 1, pp. 7–9, Jan. 2007.
- [121] E. L. Tan, "Fundamental schemes for efficient unconditionally stable implicit finite-difference time-domain methods," *IEEE Trans. Antennas Propagat.*, vol. 56, no. 1, pp. 170–177, Jan. 2008.
- [122] J. Chen and J. Wang, "PEC condition implementation for the ADI-FDTD method," *Microw. Opt. Technol. Lett.*, vol. 49, no. 3, pp. 526–530, 2007.
- [123] M. A. Rojavin and M. C. Ziskin, "Medical application of millimeter waves," *Q. J. Med.*, vol. 91, no. 1, pp. 57–66, Jan. 1998.
- [124] S. I. Alekseev and M. C. Ziskin, "Millimeter-wave absorption by cutaneous blood vessels: a computational study," *IEEE Trans Biomed. Engineering*, vol. 56, no. 10, pp. 2380–2388, Oct. 2009.
- [125] W. C. Tay, D. Y. Heh, and E. L. Tan, "GPU-accelerated fundamental ADI-FDTD with complex frequency shifted convolutional perfectly matched layer," *Progress In Electromagnetics Research M*, vol. 14, pp. 177–192, 2010.
- [126] L. Bai, L. Wang, B. Wang and J. Song, "Reverberation chamber modeling using FDTD," *IEEE Int. Symp. Electromagn. Compat.*, vol. 1, pp. 7–11, 1999
- [127] N. K. Kouveliotis, P. T. Trakadas and C. N. Capsalis, "FDTD modeling of a vibrating intrinsic reverberation chamber," *Progress In Electromagnetics Research*, vol. 39, pp. 47–59, 2003.
- [128] P. Bonnet, R. Vernet, S. Girard and F. Paladian, "FDTD modeling of reverberation chamber," *Electron. Lett.*, vol. 41, no. 20, pp. 1101–1102, Sep. 2005.

- [129] M. E. Haffar, A. Reineix, C. Guiffaut and A. Adardour, "Reverberation chamber modeling using the FDTD method," *2009 ACTEA*, pp. 151–156, 2009.
- [130] Draft IEC 61000-4-21, *Electromagnetic Compatibility (EMC) Part 4: Testing and Measurement Techniques*, Section 21, Reverberation Chambers Test Methods. 2001.
- [131] W. G. Zijlstra, A. Buursma and W. P. Meeuwssen-van der Roest, "Absorption spectra of human fetal and adult oxyhemoglobin, deoxyhemoglobin, carboxyhemoglobin, and methemoglobin," *Clin. Chem.*, vol. 37, pp. 1633–1668, 1991.
- [132] W. G. Zijlstra, A. Buursma, H. E. Falke and J. F. Catsburg, "Spectrophotometry of hemoglobin: absorption spectra of rat oxyhemoglobin, deoxyhemoglobin, carboxyhemoglobin, and methemoglobin," *Comput. Biochem. Physiol.*, vol. 107B, pp. 161–166, 1994.
- [133] W. G. Zijlstra, A. Buursma and O. W. van Assendelft, *Visible and Near Infrared Absorption Spectra of Human and Animal Haemoglobin: Determination and Application* Zeist: VSP, 2000.
- [134] M. Cope, "The application of near infrared spectroscopy to non invasive monitoring of cerebral oxygenation in the newborn infant," PhD Dissertation, 1991.
- [135] S. A. Prahl, Tabulated molar extinction coefficient for hemoglobin in water, <http://omlc.ogi.edu/spectra/hemoglobin/summary.html>, 1998.
- [136] J. G. Kim, M. Xia and H. Liu, "Extinction coefficients of hemoglobin for near-infrared spectroscopy of tissue," *IEEE Engineering in Med. and Biol. Magazine*, vol. 24, pp. 118–121, 2005.
- [137] J. G. Kim and H. Liu, "Variation of haemoglobin extinction coefficients can cause errors in the determination of haemoglobin concentration measured by near-infrared spectroscopy," *Phys. Med. Biol.*, vol. 52, pp. 6295–6332, 2007.
- [138] M. Meinke and M. Friebe, "Complex refractive index of hemoglobin in the wavelength range from 250 to 1100 nm," *Proc. SPIE*, vol. 5862, pp. 1–7, 2005.
- [139] M. Meinke and M. Friebe, "Determination of the complex refractive index of highly concentrated hemoglobin solutions using transmittance and reflectance measurements," *J. Biomed. Opt.*, vol. 10, 2005.
- [140] M. Meinke and M. Friebe, "Model function to calculate the refractive index of native hemoglobin in the wavelength range of 250 nm to 1100 nm dependent on concentration," *Appl. Opt.*, vol. 45, pp. 2838–2842, 2006.
- [141] G. M. Hale, M. R. Querry, "Optical constants of water in the 200 nm to 200 μ m wavelength region," *Appl. Opt.*, vol. 12, pp. 555–563, 1973.
- [142] B. Gustavsen and A. Semlyen, "Rational approximation of frequency domain responses by vector fitting," *IEEE Trans. Power Delivery*, vol. 14, pp. 1052–1061, 1999.
- [143] C. M. Furse and O. P. Gahdhi, "A memory efficient method of calculating specific absorption rate in CW FDTD simulations," *IEEE Trans. Biomed. Eng.*, vol. 43, pp. 558–560, 1996.

- [144] S. Paker and L. Sevgi, "FDTD evaluation of the SAR distribution in a human head near a mobile cellular phone," *Elektrik*, vol. 6, pp. 227–242, 1998.
- [145] I. Laakso, "FDTD method in assessment of human exposure to base station radiation," *Masters Dissertation*, 2007.
- [146] S. G. Garcez, C. F. Galan, L. H. Bonani and V. Baranauskas, "Estimating the electromagnetic field effects in biological tissues through the finite-difference time-domain method," *SBMO/IEEE MTT-S Int. Microw. and Optoelectronics Conf. Proc.*, vol. 43, pp. 58–62, 2007.
- [147] J. D. Jackson, *Classical Electrodynamics. 3rd Ed.*, New York: John Wiley & Sons, 1998.
- [148] D. M. Pozar, *Microwave Engineering, 3rd Ed.*, New York: Wiley, 2005.
- [149] K. Boryczko, W. Dzewinel and D. A. Yuen, "Modeling fibrin aggregation in blood flow with discrete particles," *Computer Methods and Programs in Biomedicine*, vol. 75, pp. 181–194, 2004.
- [150] P. Y. Han, G. C. Cho and X. C. Zhang, "Time-domain transillumination of biological tissues with terahertz pulses," *Opt. Lett.*, vol. 25, pp. 242–244, 2000.
- [151] S. W. Smye, J. M. Chamberlain, A. J. Fitzgerald and E. Berry, "The interaction between Terahertz radiation and biological tissue," *Phys. Med. Biol.*, vol. 46, pp. R101–112, 2001.
- [152] E. Pickwell and V. P. Wallace, "Biomedical applications of terahertz technology," *J. Phys. D: Appl. Phys.*, vol. 39, pp. R301–310, 2006.
- [153] J. -H. Son, "Terahertz electromagnetic interactions with biological matter and their applications," *J. Appl. Phys.*, vol. 105, art. no. 102033, 2009.
- [154] R. M. Woodward, B. E. Cole, V. P. Wallace, D. D. Arnold, R. J. Pye, E. H. Linfield, M. Pepper and A. G. Davies, "Terahertz pulse imaging of in vitro basal cell carcinoma samples," *TOPS*, vol. 56, pp. 329–330, 2001.
- [155] R. M. Woodward, B. E. Cole, V. P. Wallace, R. J. Pye, D. D. Arnold, E. H. Linfield and M. Pepper, "Terahertz pulse imaging in reflection geometry of human skin cancer and skin tissue," *Phys. Med. Biol.*, vol. 47, pp. 3853–3863, 2002.
- [156] E. Pickwell, B. E. Cole, A. J. Fitzgerald, M. Pepper and V. P. Wallace, "In vivo study of human skin using pulsed terahertz radiation," *Phys. Med. Biol.* vol. 49, pp. 1595–1607, 2004.
- [157] V. P. Wallace, P. F. Taday, A. J. Fitzgerald, R. M. Woodward, J. Cluff, R. J. Pye and D. D. Arnone, "Terahertz pulsed imaging and spectroscopy for biomedical and pharmaceutical applications," *Faraday Discuss.*, vol. 126, pp. 255–263, 2004.
- [158] V. P. Wallace, A. J. Fitzgerald, S. Shankar, N. Flanagan, R. J. Pye, J. Cluff and D. D. Arnone, "Terahertz pulsed imaging of basal cell carcinoma ex vivo and in vivo," *British J. Dermatol.*, vol. 151, pp. 424–32, 2004.

- [159] V. P. Wallace, A. J. Fitzgerald, E. Pickwell, R. J. Pye, P. F. Taday, N. Flanagan and H. A. Thomas, "Terahertz pulsed spectroscopy of human basal cell carcinoma," *Appl. Spectroscopy*, vol. 60, pp. 1127–1133, 2006.
- [160] E. Pickwell, B. E. Cole, A. J. Fitzgerald, V. P. Wallace and M. Pepper, "Simulation of terahertz pulse propagation in biological systems," *Appl. Phys. Lett.*, vol. 84, pp. 2190–2192, 2004.
- [161] E. Pickwell, A. J. Fitzgerald, B. E. Cole, P. F. Taday, R. J. Pye, T. Ha, M. Pepper and V. P. Wallace, "Simulating the response of terahertz radiation to basal cell carcinoma using ex vivo spectroscopy measurements," *J. Biomed. Opt.* vol. 10, art. no. 064021, 2005.
- [162] J. Sandby-Moller, T. Poulsen and H. C. Wulf, "Epidermal thickness at different body sites: relationship to age, gender, pigmentation, blood content, skin type and smoking habits," *Acta Dermatol. Venereol.* vol. 83, pp. 410–413, 2003.
- [163] M. J. Koehler, T. Vogel, P. Elsner, K. Konig, R. Buckle and M. Kaatz, "In vivo measurement of the human epidermal thickness in different localizations by multiphoton laser tomography," *Skin Research and Technology*, vol. 16, pp. 259–264, 2010.
- [164] K. Tanaka and M. Tanaka, "Simulations of nanometric optical circuits based on surface plasmon polariton gap waveguide," *Appl. Phys. Lett.*, vol. 82, no. 8, pp. 1158–1160, Feb. 2003.
- [165] S. A. Maier, P. G. Kik and H. A. Atwater, "Optical pulse propagation in metal nanoparticle chain waveguides," *Phys. Rev. B*, vol. 67, art. no. 205402, 2003.
- [166] S. A. Maier and H. A. Atwater, "Plasmonics: Localization and guiding of electromagnetic energy in metal/dielectric structures," *J. Appl. Phys.*, vol. 98, art. no. 011101, 2005.
- [167] A. Vial, A. -S. Grimault, D. Marcias, D. Barchiesi and M. L. de la Chapelle, "Improved analytical fit of gold dispersion: Application to the modeling of extinction spectra with a finite-difference time-domain method," *Phys. Rev. B*, vol. 71, pp. 085416(1)–085416(7), Feb. 2005.
- [168] P. B. Johnson and R. W. Christy, "Optical constants of the noble metal," *Phys. Rev. B*, vol. 6, pp. 4370–4379, 1972.
- [169] A. D. Rakic, A. B. Djurisic, J. M. Elazar and M. L. Majewski, "Optical properties of metallic films for vertical-cavity optoelectronic devices," *Appl. Opt.*, vol. 37, no. 22, pp. 5271–5283, Aug. 1998.
- [170] D. W. Lynch and W. R. Hunter, "Comments on the optical constants of metals and an introduction to the data for several metals," in *Handbook of Optical Constants of Solids*, E. D. Palik, Orlando Fla.: Academic, 1985.
- [171] J. Shibayama, R. Takahashi, J. Yamauchi and H. Nakano, "Frequency-dependent locally one-dimensional FDTD implementation with a combined dispersion model for the analysis of surface plasmon waveguides," *IEEE Photonics Tech. Lett.*, vol. 20, no. 10, pp. 824–826, May 2008.
- [172] Z. Han, E. Forsberg and S. He, "Surface plasmon Bragg gratings formed in metal-insulator-metal waveguides," *IEEE Photonics Tech. Lett.*, vol. 19, no. 2, pp. 91–93, Jan. 2007.

- [173] J. Shibayama, A. Nomura, R. Ando, J. Yamauchi and H. Nakano, “A frequency-dependent LOD-FDTD method and its application to the analyses of plasmonic waveguide devices,” *IEEE J. Quantum Elec.*, vol. 46, no. 1, pp. 40–49, Jan. 2010.
- [174] D. Y. Heh and E. L. Tan, “FDTD modeling for dispersive media using matrix exponential method,” *IEEE Microw. Wireless Compon. Lett.*, vol. 19, no. 2, pp. 53–55, Feb. 2009.
- [175] B. Guo, J. Li and H. Zmuda, “A new FDTD formulation for wave propagation in biological media with cole-cole model,” *IEEE Microw. Wireless Compon. Lett.*, vol. 16, no. 12, pp. 633–635, Dec. 2006.
- [176] G. Zhao and Q. H. Liu, “The unconditionally stable pseudospectral time-domain (PSTD) method,” *IEEE Microw. Wireless Compon. Lett.*, vol. 13, no. 11, pp. 475–477, Nov. 2003.
- [177] C. Ma and Z. Chen, “Dispersion analysis of the three dimensional complex envelope ADI-FDTD method,” *IEEE Trans. Antennas Propagat.*, vol. 53, no. 3, pp. 971–976, Mar. 2005.
- [178] M. S. Starosta and A. K. Dunn, “Three-dimensional computation of focus beam propagation through multiple biological cells,” *Optics Express*, vol. 17, no. 15, pp. 12455–12469, Jul. 2007.
- [179] P. Sypek, A. Dziekonski and M. Mrozowski, “How to render FDTD computations more effective using a graphics accelerator,” *IEEE Trans. Magnetics*, vol. 45, no. 3, pp. 1324–1327, Mar. 2009.
- [180] J. J. Hu, G. Ren, X. Yu, G. Wang, P. P. Shum, C. Lu, K. T. V. Grattan and T. Sun, “A generalized 2D FDTD model for photonic crystal fibers with frequency dependent media,” *Opt. Quant. Electron.*, vol. 39, no. 12-13, pp. 1133–1143, 2007.
- [181] J. A. Gordan and R. W. Ziolkowski, “CNP optical metamaterials,” *Optics Express*, vol. 16, no. 9, pp. 6692–6716, Apr. 2008.